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Multi-phonon processes in slow neutron scattering by crystals

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With 12 figures in the text

ABSTRACT

The multi-phonon processes in incoherent scattering of slow neutrons by crystals are discussed, assuming the harmonic approximation for the crystal vibrations. The differential scattering cross section is expanded in the Hermite orthogonal functions and approximate expressions for the cross section are derived. Extensive numerical calculations have been carried out to illustrate the accuracy of the approximations made. An approximation for the total cross section (the mass-ratio expansion) suggested by Placzek is discussed and in some respects generalized. The approximations for the differential cross section mentioned above are also used to derive approximate formulae for the total cross section valid for cold neutrons but arbitrary temperatures and mass ratios.

Introduction

The basic ideas of the theory of slow neutron scattering by crystals were developed by Wick [1], Pomeranchuk [2], Seeger and Teller [3] and Akhieser and Pomeranchuk [4]. A quantitative account was given by Weinstock [5], who discussed the temperature dependence of the total scattering. Afterwards the formal treatment was completed especially by Fröman [6]. He separated the scattering into phonon processes and consistently used the analogies with X-ray diffraction. An alternative method, very convenient for calculating the total scattering cross section, was later suggested by Placzek [7]. Recently the theory was reformulated by Glauber [8] and Van Hove [9] making it more surveyable. They derived closed expressions for the differential scattering cross section, which seem to be a convenient starting point for quantitative discussions. Van Hove also generalized the theory to general systems of nuclei, as for instance liquids and magnetic materials. A large number of experiments have been performed and these mainly confirm the basis of the theoretical treatment [10–19]. Though the formal treatment seems to be fairly complete no complete quantitative investigations have been made. Some important aspects have been thoroughly discussed, as for instance one-phonon scattering [20–25] and total scattering [7, 26–29], but no satisfactory treatment of the multi-phonon processes is given [30, 34]. Especially in recent years great progress has been made in getting detailed information on the vibrational properties of a crystal [14–18, 31–33] and therefore it would be of importance to conclude from theory how the scattering should depend on the detailed properties of the crystal vibrations. In cases where the details give no significant effects it is important to know more precisely what average property of the vibrations is found from the scattering data. In this paper and an earlier one [34] these aspects of the problem have been discussed and where justified simplifying approximations have been made to get more simple expressions for the scattering cross sections.

In part I a brief account of the theoretical background is given. In part II the energy distribution of the scattered neutrons in different scattering directions is investigated and in part III the total cross section is treated. When dealing with the high-phonon processes it seems to be convenient to separate the scattering into an incoherent part and an interference part, where these two should be treated in rather different ways. In parts II and III only the incoherent part of the scattering is treated.

PART I

GENERAL THEORY

Chapter 1. Crystal dynamics

A rigorous theory of the thermal vibrations in a real crystal would be very involved because of several physical effects which complicate the mathematical treatment while having little bearing on the case considered here. In order to obtain a simplified description of the vibrational states in the crystal we will therefore from the start disregard some aspects and concentrate on the important features. We consider the crystal as perfect, apart from thermal displacements, and neglect all surface distortions of the vibrations. In addition we adopt the harmonic approximation for the vibrational potential. On these assumptions the general state of motion of the nuclei can be represented as a superposition of plane waves, each of which is characterized by its wave vector $\mathbf{q}$, frequency ω and polarization vector $\mathbf{C}^k$.

An account of elements of the dynamical theory of crystals can be found in the textbooks and review articles referred to [35–38]. Here we only explain the notations to be used and write the formulae needed in the following. As usual we specify the position vector of a nucleus by the lattice vector $\mathbf{R}^l$, where $l=(l_1, l_2, l_3)$ are the cell indices, by the equilibrium position vector in an elementary cell $\mathbf{r}_k$ ($k=1, 2, \ldots, n$, where n is the number of nuclei in an elementary cell) and by the displacement vector $\mathbf{u}_k^l$. The origin is placed at a nucleus within the crystal and the instantaneous position of any nucleus is then specified by $\mathbf{r}_k^l=\mathbf{R}^l+\mathbf{r}_k+\mathbf{u}_k^l$.

Separating the motion of the nuclei in plane waves we may write (¹)

$$\mathbf{u}_k^l=\sum_{j\mathbf{q}}\left(\frac{\hbar}{2NM_k\omega_j}\right)^{\frac{1}{2}}\mathbf{C}_j^k(\mathbf{q})\left[a_{j\mathbf{q}}e^{i(\mathbf{q}\cdot\mathbf{R}^l-\omega_j t)}-a_{j-\mathbf{q}}^{+}e^{i(\mathbf{q}\cdot\mathbf{R}^l+\omega_j t)}\right] \tag{I.1}$$

with $\mathbf{C}_j^{k*}(-\mathbf{q})=-\mathbf{C}_j^k(\mathbf{q})$ and $\omega_j(\mathbf{q})=\omega_j(-\mathbf{q})$ $(j=1, 2, \ldots, 3n)$.

(¹) See also: R. J. Glauber, Phys. Rev., *98*, 1692 (1955).

Here each eigenstate has been labelled by the double index $(\mathbf{q}j)$. N is the number of unit cells in the crystal and M_k denotes the mass of the kth nucleus. $a_{j\mathbf{q}}$ and the Hermitian conjugated one $a_{j\mathbf{q}}^{+}$ are respectively the annihilation and creation operators concerned with the harmonic oscillator. They must fulfill the commutation relations below

$$\left.\begin{aligned} a_s a_{s'} - a_{s'} a_s &= 0 \\ a_s a_{s'}^{+} - a_{s'}^{+} a_s &= \delta_{ss'} \end{aligned}\right\} \quad s = (\mathbf{q}j). \tag{I.2}$$

The eigenfrequencies and polarization vectors are determined from a system of equations

$$\omega^2 C_x^k = \sum_{k'y} \mathcal{D}_{xy}^{kk'} C_y^{k'}, \tag{I.3}$$

where the dynamical matrix $\mathcal{D}_{xy}^{kk'}$ (¹) is related to the interatomic forces in the crystal and the wave vector $\mathbf{q}$ by

$$\mathcal{D}_{xy}^{kk'} = \sum_{l} \mathcal{V}_{xy}^{kk'}(l)\, e^{i\mathbf{q}\cdot\mathbf{R}^l}, \tag{I.4}$$

$\mathcal{V}_{xy}^{kk'}(l)$ being force constants. $\mathbf{C}^k$ are ortho-normalized as follows:

$$\left.\begin{aligned} \sum_{k,x} C_{j\mathbf{q},x}^{k*} C_{j'\mathbf{q},x}^{k} &= \delta_{jj'}, \\ \sum_{j} C_{j\mathbf{q},x}^{k*} C_{j\mathbf{q},y}^{k'} &= \delta_{kk'}\,\delta_{xy'}. \end{aligned}\right\} \tag{I.5}$$

The wave vectors are restricted to N discrete values, and if drawn in the reciprocal lattice they will uniformly fill a unit cell. Now N is supposed to be very large and therefore a summation over $\mathbf{q}$ can be replaced by an integration over the reciprocal unit cell. For the same reason it is convenient to introduce the density function $f(\omega)$ defined in the following way:

$f(\omega)\,d\omega =$ the number of eigenstates in the frequency interval $(\omega, \omega + d\omega)$ divided by the total number of eigenstates $3nN$.

As shown by Van Hove [39] and Phillips [40] $f(\omega)$ is continuous and its derivative has a certain number of isolated singularities.

To each eigenstate corresponds a mean energy

$$\varepsilon_s = \frac{\hbar\omega_s}{2}\coth(\beta\omega_s), \qquad \beta = \frac{\hbar}{2k_B T}, \tag{I.6}$$

where T is the temperature of the crystal and k_B is Boltzmann's constant, and thus the total vibrational energy per nucleus may be written

$$E_c = 3\int_0^{\omega_m} \frac{\hbar\omega}{2}\coth(\beta\omega)\, f(\omega)\, d\omega, \tag{I.7}$$

where ω_m is the maximum vibrational frequency.

(¹) See: M. Born, Reports Progr. Phys., vol. IX, 294 (1943).

All discussions of the neutron scattering can be based on the time correlation function $\mathcal{M}^l_{kk'}(t) = \langle \mathbf{u}^0_{k'}(0)\, \mathbf{u}^l_k(t)\rangle_T$, where $\langle \cdots \rangle_T$ is the statistical expectation value at temperature T. Using the commutation relations (I.2) and further (I.6) it is a straightforward matter to derive the following expression

$$\boxed{\mathcal{M}^l_{\substack{kk'\\xy}} = \langle u^0_{k',x}(0)\, u^l_{k,y}(t)\rangle_T = \frac{\hbar}{2N(M_k M_{k'})^{\frac{1}{2}}} \sum_s g_s(t)\, C^{k'*}_{s,x}\, C^k_{s,y}\, e^{i\mathbf{q}\cdot\mathbf{R}^l},} \tag{I.8}$$

where
$$g_s(t) = \coth(\beta\omega_s)\frac{\cos(\omega_s t)}{\omega_s} + i\,\frac{\sin(\omega_s t)}{\omega_s}. \tag{I.9}$$

For crystals with cubic structure the tensor $\mathcal{M}^0_{kk}$ simplifies to a scalar times the unit tensor(¹) and if further restricting ourselves to those crystals which constitute a simple Bravais lattice we may write

$$\mathcal{M}^0(t) = \mathcal{J}\frac{\hbar}{2M}\int_0^{\omega_m} [\coth(\beta\omega)\cos(\omega t) + i\sin(\omega t)]\frac{f(\omega)}{\omega}\,d\omega, \tag{I.10}$$

$\mathcal{J}$ being the unit tensor.(²) The index k is now unnecessary and therefore omitted in the expression above. We note that all properties of the crystal are contained in the frequency function $f(\omega)$ and the maximum frequency ω_m.

Chapter 2. Differential scattering cross section

To account for the scattering of neutrons Fermi's pseudo-potential [41] is introduced to represent the interaction between the neutron and a single nucleus. Generally we must distinguish between scattering with parallel and antiparallel spins of the neutron and the nucleus. We can account for both possibilities by introducing a spin-dependent pseudo-potential

$$V' = -\frac{2\pi\hbar^2}{m}(\alpha + 2\alpha'\,\mathbf{S}\cdot\mathbf{s})\,\delta(\mathbf{r}-\mathbf{R}). \tag{I.11}$$

Here $\mathbf{r}$ and $\mathbf{s}$ denote the position vector and spin vector of the neutron, the latter in units of $\hbar$, and $\mathbf{R}$ and $\mathbf{S}$ denote the corresponding quantities for the nucleus. m is the neutron mass and (³)

$$\left.\begin{aligned} \alpha &= \frac{j+1}{2j+1}a_+ + \frac{j}{2j+1}a_-, \\ \alpha' &= \frac{1}{2j+1}(a_+ - a_-), \end{aligned}\right\} \tag{I.12}$$

(¹) We may draw the more general conclusion that the tensor $\mathcal{M}^0_{kk}$ has the same symmetry as the crystal structure.

(²) The scalar factor will later be denoted by $\frac{\hbar}{2M}\gamma(t)$.

(³) See for instance: L. Rosenfeld, Nuclear Forces, Amsterdam 1948, p. 106.

where j is the spin and a_+ and a_- are the scattering lengths for the bound nucleus referred to parallel and antiparallel spins respectively.

If the study is restricted to non-magnetic materials (1) the interaction between the neutron and the whole crystal is obtained by summing the single nucleus potential (I.11) over all nuclei. We must then label quantities depending on the kind of nucleus by the index $(l\,k)$.(2)

We get

$$\left.\begin{aligned} V &= -\frac{2\pi\hbar^2}{m}\sum_{lk} O_{lk}\,\delta(\mathbf{r}-\mathbf{r}_k^l),\\ O_{lk} &= \alpha_{lk} + 2\,\alpha'_{lk}\,(\mathbf{S}_{lk}\cdot\mathbf{s}). \end{aligned}\right\} \qquad \text{(I.13)}$$

With Born's approximation for solving the scattering problem the integration over the neutron space coordinates gives the following expression for the differential scattering cross section

$$\frac{d^2\sigma}{d\Omega\,d\omega} = \frac{k}{k_0}\sum_n\sum_{n_0} p_{n_0}\,|(n\,|F|\,n_0)|^2\,\delta(\omega-\omega_0+\omega_{nn_0}). \qquad \text{(I.14)}$$

The summation is extended over the final states $|n)$ and the initial states $|n_0)$ of the crystal, the latter weighted by the statistical factor p_{n_0}. The summation should also include the spin states of the neutron. Further the following notations are used:

$\omega = E/\hbar$, $\omega_0 = E_0/\hbar$, where E and E_0 are the energies of the scattered and incoming neutron respectively.
E_n = energy of the final vibrational state.
E_{n_0} = energy of the initial vibrational state.
$\omega_{nn_0} = (E_n - E_{n_0})/\hbar$.

The δ-function assures the energy conservation. $(n\,|F|\,n_0)$ is the transition matrix and F is given by

$$F = \sum_{lk} O_{lk}\exp\,(i\,\boldsymbol{\varkappa}\cdot\mathbf{r}_k^l)$$

and $\boldsymbol{\varkappa} = \mathbf{k}_0 - \mathbf{k}$, $\mathbf{k}_0$ and $\mathbf{k}$ are the wave vectors of the incoming and scattered neutron.

The scattering cross section can be simplified by introducing a time-dependent pair-distribution function [8, 9]. Since we proceed in a similar way as the authors referred to a presentation of the details seems to be redundant. We account for both the spin dependence of the scattering and the isotopic disorder in the crystal.

The δ-function in (I.14) is first written as a Fourier integral

$$\delta(\omega-\omega_0+\omega_{nn_0}) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\,[i\,(\omega-\omega_0)\,t]\,\exp\,[i\,(E_n-E_{n_0})\,t/\hbar]\,dt$$

and further

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(1) The non-magnetic interaction between electrons and neutrons is neglected.

(2) Compare the notation of the positions of the nuclei in the foregoing chapter.

$$\exp\,[i\,(E_n - E_{n_0})\,t/\hbar]\,(n\,|\,F\,|\,n_0) = \left(n\,\middle|\,\exp\left(\frac{i\,t\,H}{\hbar}\right) F \exp\left(\frac{-\,i\,t\,H}{\hbar}\right)\middle|\,n_0\right),$$

where H denotes the Hamiltonian of the system of nuclei, supposed not to contain any spin variable.

$$\exp\left(\frac{i\,t\,H}{\hbar}\right) F \exp\left(\frac{-\,i\,t\,H}{\hbar}\right)$$

may be considered as a Heisenberg observable which can also be written (¹)

$$F\,(t) = \sum_{lk} 0_{lk} \exp\,[i\,\boldsymbol{\varkappa}\cdot\mathbf{r}_k^l\,(t)]. \tag{I.15}$$

The differential scattering cross section is now transformed as follows:

$$\frac{d^2\sigma}{d\Omega\,d\omega} = \frac{k}{k_0}\,\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\,[i\,(\omega-\omega_0)\,t]\,dt\,\{\sum_n \sum_{n_0} p_{n_0}\,(n_0\,|\,F^+\,(0)\,|\,n)\,(n\,|\,F\,(t)\,|\,n_0)\} =$$

$$= \frac{k}{k_0}\,\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\,[i\,(\omega-\omega_0)\,t]\,dt\,\langle F^+\,(0)\,F\,(t)\rangle_T. \tag{I.16}$$

The completeness of the eigenfunctions has been used to perform the summation over $|\,n)$, including the spin states of the scattered neutrons. The second summation is contained in the definition of the statistical average value. As shown below this is independent of the spin states of the incoming neutron and thus the summation over the initial neutron spin states only gives a factor of unity.

We further note that

$$\langle \mathbf{S}_{lk}\cdot\mathbf{s}\rangle_T = \langle(\mathbf{S}_{lk}\cdot\mathbf{s})^+\rangle_T = 0, \qquad \langle(\mathbf{S}_{lk}\cdot\mathbf{s})^+\,(\mathbf{S}_{l'k'}\cdot\mathbf{s})\rangle_T = \tfrac{1}{4}\,j_{lk}\,(j_{lk}+1)\,\delta_{ll'}\,\delta_{kk'}.$$

and if using these relations

$$\langle 0_{lk}^+\,0_{l'k'}\rangle_T = \alpha_{lk}\,\alpha_{l'k'} + \alpha_{lk}'^2\,j_{lk}\,(j_{lk}+1)\,\delta_{ll'}\,\delta_{kk'}. \tag{I.17}$$

By separating the spin states and space states of the crystal and putting the expression for $F\,(t)$ in (I.15) into (I.16) this can be simplified further. To save space we introduce the notation

$$G_{kk'}^{ll'} = \langle \exp\,[-\,i\,\boldsymbol{\varkappa}\cdot\mathbf{r}_k^l\,(0)]\,\exp\,[i\,\boldsymbol{\varkappa}\cdot\mathbf{r}_{k'}^{l'}\,(t)]\rangle_T. \tag{I.18}$$

We can then write

$$\langle F^+\,(0)\,F\,(t)\rangle_T = \sum_{lk}\sum_{l'k'} \alpha_{lk}\,\alpha_{l'k'}\,G_{kk'}^{ll'} + \sum_{lk} \alpha_{lk}'^2\,j_{lk}\,(j_{lk}+1)\,G_{kk}^{ll}. \tag{I.19}$$

(¹) The symbol t then has the physical meaning of a time. Cf. L. Van Hove, Phys. Rev., *95*, 249 (1954).

For mono-isotopic nuclei we may drop the index l in α_{lk} and α'_{lk}. When there are several isotopes of a certain kind of nucleus we instead define the mean values, $\langle\alpha_k\rangle$ for instance, over the different isotopes with regard to the abundance.(1)

Owing to the assumption of complete isotopic disorder and the equivalence of all lattice points (2) it can be shown that

$$\sum_{lk}\sum_{l'k'}\alpha_{lk}\,\alpha_{l'k'}\,G^{ll'}_{kk'}=N\sum_{kk'}\langle\alpha_k\rangle\langle\alpha_{k'}\rangle\,(\sum_{l}G^{0l}_{kk'})+N\sum_{k}(\langle\alpha_k^2\rangle-\langle\alpha_k\rangle^2)\,G^{00}_{kk}$$

and analogously for the second term in (I.19). By further using (I.12) we get

$$\langle F^{+}(0)\,F(t)\rangle_T=N\sum_{kk'}\langle a_k\rangle\langle a_{k'}\rangle\,(\sum_{l}G^{0l}_{kk'})+N\sum_{k}(\langle a_k^2\rangle-\langle a_k\rangle^2)\,G^{00}_{kk}, \qquad \text{(I.20)}$$

where $\langle a_k\rangle$ and $\langle a_k^2\rangle$ are respectively the mean values of the scattering length and its square, averaged over the two spin states and all isotopes.

The scattering is in this way separated into two terms, the coherent part, which includes all interference effects, and the incoherent part, which has the character of one-nucleus scattering.

As shown by Van Hove [9] and Glauber [8] we can finally rewrite $G^{0l}_{kk'}$ in the following form (3)

$$G^{0l}_{kk'}=\exp\left[-\tfrac{1}{2}\,\boldsymbol{\varkappa}\cdot\mathfrak{M}^{0}_{kk}(0)\cdot\boldsymbol{\varkappa}-\tfrac{1}{2}\,\boldsymbol{\varkappa}\cdot\mathfrak{M}^{0}_{k'k'}(0)\cdot\boldsymbol{\varkappa}+\boldsymbol{\varkappa}\cdot\mathfrak{M}^{l}_{kk'}(t)\cdot\boldsymbol{\varkappa}\right] \qquad \text{(I.21)}$$

Using (I.20) and (I.21) we get from (I.16) the following expression for the differential scattering cross section per unit cell, separated into the coherent and the incoherent part:

$$\boxed{\frac{d^2\sigma_{\text{incoh}}}{d\Omega\,d\omega}=\frac{k}{k_0}\sum_{k}A_k\exp[-\boldsymbol{\varkappa}\cdot\mathfrak{M}^{0}_{kk}(0)\cdot\boldsymbol{\varkappa}]\,\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\,[i(\omega-\omega_0)t]\,\exp\,[\boldsymbol{\varkappa}\cdot\mathfrak{M}^{0}_{kk}(t)\cdot\boldsymbol{\varkappa}]\,dt,}$$

(I.22 a)

$$\boxed{\begin{aligned}\frac{d^2\sigma_{\text{coh}}}{d\Omega\,d\omega}=\frac{k}{k_0}\sum_{kk'}\langle a_k\rangle\langle a_{k'}\rangle\,\exp\,[i\boldsymbol{\varkappa}\cdot(\mathbf{r}_{k'}-\mathbf{r}_k)]\,\exp\,[-\tfrac{1}{2}\,\boldsymbol{\varkappa}\cdot\mathfrak{M}^{0}_{kk}(0)\cdot\boldsymbol{\varkappa}-\\ -\tfrac{1}{2}\,\boldsymbol{\varkappa}\cdot\mathfrak{M}^{0}_{k'k'}(0)\cdot\boldsymbol{\varkappa}]\,\sum_{l}e^{i\boldsymbol{\varkappa}\cdot\mathbf{R}^{l}}\,\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\,[i(\omega-\omega_0)t]\,\exp\,[\boldsymbol{\varkappa}\cdot\mathfrak{M}^{l}_{kk'}(t)\cdot\boldsymbol{\varkappa}]]\,dt.\end{aligned}}$$

(I.22 b)

Here $A_k=\langle a_k^2\rangle-\langle a_k^2\rangle$.

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(1) The mass difference between the isotopes causes a distortion of the plane waves in the crystal and therefore we must assume that isotopes with large mass differences are rare.

(2) The equivalence is fulfilled only if surface effects of the crystal are neglected.

(3) The proof is based on the assumption that the anharmonic effects on the crystal vibrations can be neglected. The tensors $\mathfrak{M}^{l}_{kk'}$ were defined in chapter 1.

The phonon expansion of the scattering cross section, in which each term contains processes where a fixed number of vibrational quanta participate, is obtained from (I.22 a, b) if $\exp(\boldsymbol{\varkappa}\cdot\mathcal{M}^{l}_{kk'}(t)\cdot\boldsymbol{\varkappa})$ is written as a power series. The integration over t is then easily performed and the summation over l leads to generalized δ-functions, periodic in the reciprocal lattice as

$$\delta_P(\boldsymbol{\varkappa})=\sum_{\boldsymbol{\tau}}\delta(\boldsymbol{\varkappa}-\boldsymbol{\tau}). \tag{I.23}$$

$\boldsymbol{\tau}$ is a reciprocal lattice vector defined in such a way that $(\boldsymbol{\tau}\cdot\mathbf{R}^{l})$ is a multiple of 2π. $\delta_P(\boldsymbol{\varkappa})$ is connected with the l-summation by

$$\sum_{l} e^{i\boldsymbol{\varkappa}\cdot\mathbf{R}^{l}}=\frac{(2\pi)^3}{V}\,\delta_P(\boldsymbol{\varkappa}), \tag{I.24}$$

where V means the volume of a unit cell in ordinary space.

For surveyability we only consider a Bravais lattice and then we get the following expression for zero-, one- and two-phonon terms [6]:

$$\begin{aligned}\frac{d^2\sigma_{\mathrm{coh}}}{d\Omega\,d\omega}=\langle a^2\rangle\frac{k}{k_0}\frac{(2\pi)^3}{V}\exp\left[-\boldsymbol{\varkappa}\cdot\mathcal{M}^{0}(0)\cdot\boldsymbol{\varkappa}\right]\Bigg[\delta_P(\boldsymbol{\varkappa})\,\delta(\omega-\omega_0)+\\ +\sum_{s\varepsilon}\frac{\hbar\,|\boldsymbol{\varkappa}\cdot\mathbf{C}_s|^2}{2NM\omega_s}\,\frac{\coth(\beta\omega_s)+\varepsilon}{2}\,\delta_p(\boldsymbol{\varkappa}+\mathbf{q}_s)\,\delta(\omega-\omega_0+\varepsilon\omega_s)+\\ +\frac{1}{2}\sum_{ss'\varepsilon\varepsilon'}\frac{\hbar\,|\boldsymbol{\varkappa}\cdot\mathbf{C}_s|^2}{2NM\omega_s}\,\frac{\hbar\,|\boldsymbol{\varkappa}\cdot\mathbf{C}_{s'}|^2}{2NM\omega_{s'}}\,\frac{\coth(\beta\omega_s)+\varepsilon}{2}\,\frac{\coth(\beta\omega_{s'})+\varepsilon'}{2}\times\\ \times\delta_P(\boldsymbol{\varkappa}+\mathbf{q}_s+\mathbf{q}_{s'})\,\delta(\omega-\omega_0+\varepsilon\omega_s+\varepsilon'\omega_{s'})+\cdots\Bigg],\end{aligned} \tag{I.25}$$

$\varepsilon=\pm 1$ corresponding to emission and absorption of phonons respectively, and summation should be performed over both values. $\exp(-\boldsymbol{\varkappa}\cdot\mathcal{M}^{0}(0)\cdot\boldsymbol{\varkappa})$ is the Debye-Waller factor and will also be denoted by the more common notation e^{-2W}. The incoherent cross section is obtained from (I.25) if unity is substituted for

$$\frac{(2\pi)^3}{V}\,\delta_P(\ldots)$$

and A for $\langle a^2\rangle$.

Chapter 3. Total scattering cross section

Most of the earlier investigations on neutron diffraction were concerned with the total scattering cross section. In the first calculation to obtain the temperature dependence of this cross section Weinstock [5] only considered zero- and one-phonon processes. Later Squires [11] derived approximate formulae for multi-phonon processes of any order, which he compared with available experimental results. These show that in many cases a great number of terms in the phonon expansion are required to give enough accuracy. In several papers Placzek [7] has subsequently suggested that it would be more convenient to expand the total cross section in powers of m/M, m being the neutron mass and M the nucleus mass. In this way he obtained simple formulae for the incoherent cross section, applicable to large and small neutron energies. In another paper Placzek and collaborators [27] also show how to correct for the interference effects when dealing with rather high neutron energies. Later Kothari and Singwi [26] used the m/M expansion for the inference terms as well.

It is possible to make an exact integration of the differential scattering cross sections (I.22 a, b). We need only consider the coherent part; the incoherent cross section is then obtained as a special case of the coherent one.

To abbreviate the notations we write

$$\begin{aligned}\mathbf{R} &= \mathbf{R}^l + \mathbf{r}_{k'} - \mathbf{r}_k,\\ \mathcal{M} &= \tfrac{1}{2}\,\mathcal{M}^0_{kk}(0) + \tfrac{1}{2}\,\mathcal{M}^0_{k'k'}(0) - \mathcal{M}^l_{kk'}(t).\ (^1)\end{aligned} \tag{I.26}$$

Then we get from (I.22 b)

$$\sigma_{\mathrm{coh}} = \sum_l \sum_{kk'} \langle a_k\rangle \langle a_{k'}\rangle \frac{1}{2\pi k_0} \int \exp\left[i(\omega-\omega_0)t\right] dt \left\{e^{i\boldsymbol{\varkappa}\cdot\mathbf{R}} \exp\left[-\boldsymbol{\varkappa}\cdot\mathcal{M}\cdot\boldsymbol{\varkappa}\right] k\, d\Omega\, d\omega\right\} =$$

$$= \sum_l \sum_{kk'} \langle a_k\rangle \langle a_{k'}\rangle \frac{\hbar}{2\pi m k_0} \int dt \left\{\exp\left[i\boldsymbol{\varkappa}\cdot\left(\mathbf{R} - \frac{\hbar t}{m}\mathbf{k}_0\right)\right]\cdot\right.$$

$$\left.\cdot\exp\left[-\boldsymbol{\varkappa}\cdot\left(\mathcal{M} - i\frac{\hbar t}{2m}\mathcal{J}\right)\cdot\boldsymbol{\varkappa}\right] d\boldsymbol{\varkappa}\right\} =$$

$$= \frac{\hbar\pi^{3/2}}{m k_0} \sum_l \sum_{kk'} \langle a_k\rangle \langle a_{k'}\rangle \frac{1}{2\pi} \int_{-\infty}^{\infty} \|\mathcal{B}\|^{\frac{1}{2}} \exp\left[-\tfrac{1}{4}(\mathbf{R}'\cdot\mathcal{B}\cdot\mathbf{R}')\right] dt,$$

where

$$\mathbf{R}' = \mathbf{R} - \frac{\hbar t}{m}\mathbf{k}_0, \quad \mathcal{B}^{-1} = \mathcal{M} - i\frac{\hbar t}{2m}\mathcal{J}$$

and $\|\mathcal{B}\|$ means the determinant of $\mathcal{B}$.

For surveyability we specialize to a Bravais lattice. We then get the following expression for the total scattering cross section [42]:

$$\boxed{\sigma_{\mathrm{incoh}} = A\left(\frac{\pi}{\omega_0}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left[-\frac{\hbar t^2}{2m}\mathbf{k}_0\cdot(\Gamma^0 - it\mathcal{J})^{-1}\cdot\mathbf{k}_0\right] \frac{dt}{(\|\Gamma^0 - it\mathcal{J}\|)^{\frac{1}{2}}},} \tag{I.27 a}$$

$$\boxed{\begin{aligned}\sigma_{\mathrm{coh}} = \langle a^2\rangle \left(\frac{\pi}{\omega_0}\right)^{\frac{1}{2}} \sum_l \int_{-\infty}^{\infty} \exp\left[-\frac{\hbar}{2m}\left(\frac{m}{\hbar}\mathbf{R}^l - t\mathbf{k}_0\right)\cdot(\Gamma^l - it\mathcal{J})^{-1}\cdot\left(\frac{m}{\hbar}\mathbf{R}^l - t\mathbf{k}_0\right)\right]\cdot\\ \cdot\frac{dt}{(\|\Gamma^l - it\mathcal{J}\|)^{\frac{1}{2}}}.\end{aligned}} \tag{I.27 b}$$

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(1) We may always consider $\mathcal{M}$ symmetric.

Here
$$\Gamma^{l} = \frac{2m}{\hbar}\left(\mathcal{M}^{0}(0) - \mathcal{M}^{l}(t)\right).$$

At a later stage we will specialize further to cubic lattices and then

$$\Gamma^{0} = \mathcal{J}\frac{m}{M}\int_{0}^{\omega_m}\left[\coth(\beta\omega)\left(1-\cos(\omega t)\right) - i\sin(\omega t)\right]\frac{f(\omega)}{\omega}\,d\omega. \tag{I.28}$$

The integrands in (1.27) are singular for $t=0$ when $l=0$ and some caution is therefore necessary. It is possible to avoid the difficulties by putting

$$\exp\left[i(\omega-\omega_0)t\right] \rightarrow \exp\left[i(\omega-\omega_0)(t+i\varepsilon)\right], \quad \varepsilon > 0$$

in the proof and after the t-integration let $\varepsilon \rightarrow 0$.

Chapter 4. Discussion

The derivation of the formulae for the scattering cross sections may appear to be very general. Nevertheless there are some limitations which must be emphasized.

Firstly the harmonic approximation of the vibrational motion of the nuclei is not justified for high temperatures. It is certainly possible to account for the thermal expansion of the crystal, at least in principle, by considering the nuclei to vibrate around their equilibrium position at any temperature. The interatomic forces are then supposed to be temperature-dependent and, for instance, the frequency function will vary with the temperature. It should also be mentioned that for metals the basis of the theory of the nuclear vibrations is not all clear.

The influence of the anharmonic forces in the crystal may be divided into two different effects. The first effect manifests itself through an expansion of the crystal still keeping the harmonic nature of the motion and the formalism above will be unchanged. In consequence of the other effect the plane waves are not exactly eigenstates of the crystal and we must suppose an interaction between the separate phonons, which thus have finite lifetimes. Such an interaction is also due to other effects as for instance crystal imperfections. Among other things this effect prevents the energy-momentum relation for the one-phonon scattering (see formula (I.25)) from being exactly fulfilled and causes a broadening of the in the ideal case discrete energies of the scattered neutrons. Nevertheless it is interesting to know the results in the harmonic approximation even when the assumption that the anharmonic forces are negligible is not completely justified.

The other limitation to be mentioned concerns the Bragg scattering. To obtain accurate values on the intensity of the Bragg peaks we must, except for very small single crystals, account for primary extinction, and this can only be done by using the much more complicated dynamical theory of scattering [43, 44]. Now it is possible to separate the Bragg scattering from the other scattering, both theoretically and experimentally. When dealing with the total scattering cross section polycrystal materials are often used, where extinction effects can be neglected. Except for the coherent elastic part the influence of the extinction effects on the results should be very slight.

The one-phonon scattering intensities, both coherent and incoherent, are very sensitive to the detailed vibrational properties of the crystal [22–24]. Any rough approximation of the eigenvibrations, such as the Debye approximation, would therefore fail to exhibit many of the most characteristic features of the one-phonon scattering. It is moreover possible to perform calculations on this scattering by using more realistic assumptions. As shown by the author in another paper [34] the coherent two-phonon scattering cross section, too, is rather sensitive to the details of the vibrational properties. The higher phonon terms, however, are much less sensitive to the details, and the interference terms in the coherent scattering cross section $(l \neq 0)$ make only a rather small contribution to the scattering.

We note that the term corresponding to $l=0$ and $k=k'$ in the coherent cross section is equal to the incoherent cross section apart from a numerical factor. In this paper we restrict ourselves to this term (incoherent approximation) leaving the interference part for a separate investigation.

PART II

DIFFERENTIAL SCATTERING CROSS SECTION

Chapter 1. The Doppler effect

Cubic Bravais lattices (1)

The characteristic features of the scattering are very different for "large and small neutron energies" (2) and therefore especially the latter of these two extreme cases will be discussed before passing on to intermediate energies.

For "small energies" the zero- and one-phonon terms (see formula I.25) give the main part of the scattering, the remaining terms only causing a weak and smooth background. In the case of "large energies", on the other hand, many phonon terms contribute appreciably and here the nuclei may be considered free, having a prescribed momentum distribution. The deviation of the scattering from that of fixed nuclei should thus mainly be due to the Doppler effect.(3)

The zero- and one-phonon scattering have been thoroughly investigated in other papers [20–24] and therefore we need not discuss them further. The other extreme case has also been treated before [4, 8] but will be considered in more detail.

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(1) The cubic Bravais lattices are the simple cubic, the body-centered cubic and the face-centered cubic lattices.

(2) This should mean a division into large and small values compared with unity of $2\,W = \langle(\boldsymbol{\varkappa}\cdot\mathbf{u}_k^l)^2\rangle_T$, which denotes the mean square displacement along $\boldsymbol{\varkappa}$ of a nucleus multiplied by $\varkappa^2$. The neutron energies considered in practice extend from some few eV down to about 10^{-4} eV.

(3) It should not be assumed that the interference effect on the coherent scattering is negligible for large neutron energies. On the contrary, Placzek and collaborators [7, 27] have shown that for the total scattering cross section the interference correction will for heavy nuclei exceed the Doppler correction.

For convenience all frequencies appearing in the following will be measured in units of the maximum vibrational frequency ω_m and the time in units of $1/\omega_m$.

Thus, for instance,
$$Q = \frac{\hbar \varkappa^2}{2M} \quad \text{and} \quad \beta = \frac{\hbar}{2 k_B T} \tag{II.1}$$

are dimensionless quantities.

The differential scattering cross section was given in (I.22 a) and for a cubic Bravais lattice this expression simplifies to

$$\frac{d^2 \sigma_{\text{incoh}}}{d\Omega \, d\omega} = A \frac{k}{k_0} \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\,[i(\omega - \omega_0)t] \exp\,(Q[\gamma(t) - \gamma(0)])\, dt, \tag{II.2}$$

where
$$\gamma(t) = \int_0^1 \left[\coth(\beta\zeta) \cos(\zeta t) + i \sin(\zeta t)\right] \frac{f(\zeta)}{\zeta}\, d\zeta \tag{II.3}$$

depends on the vibrational properties only by the frequency function $f(\zeta)$.

$Q\gamma(0) = 2W$ is the ordinary Debye–Waller function and when

$$2W \gg 1$$

the region near $t=0$ makes the main contribution to the integral and therefore $\gamma(t)$ may be expanded in powers of t, neglecting in the first approximation third and higher order terms.

$$\gamma(t) - \gamma(0) = it - \frac{2}{3} \frac{E_{\text{kin}}}{\hbar} t^2 + \cdots. \tag{II.4}$$

$E_{\text{kin}} = E_c/2$ is then the mean kinetic energy per nucleus.

In this approximation, henceforth called the Doppler approximation, the time integration in easily performed and gives the result:

$$\boxed{\frac{d^2 \sigma_{\text{incoh}}}{d\Omega \, d\omega} = A \frac{k}{k_0} \frac{(2\pi)^{-\frac{1}{2}}}{\Delta} \exp\left[-\frac{(\omega - \omega_0 + Q)^2}{2\Delta^2}\right],} \tag{II.5}$$

where
$$\Delta^2 = \frac{4Q}{3} \frac{E_{\text{kin}}}{\hbar}. \tag{II.5$'$}$$

For high temperatures E_{kin} approaches the value $3 k_B T/2$ corresponding to the kinetic energy per nucleus for a Maxwellian gas of free nuclei. The scattering will be approximately the same as for neutrons scattered against such a nuclear gas.(¹)

(¹) Cf.: B. N. Brockhouse, D. J. Hurst, Phys. Rev. *88*, 542 (1952), formula (5).

As shown by Brockhouse and Hurst [13] this free gas model gives a fairly good interpretation of their experimental results on lead and aluminium at the neutron wavelength 0.48 Å ($E = 0.35$ eV). In (II:5) the model is completed in as far as the actual momentum distribution of the nuclei in the crystal is inserted, a fact which is proved in Appendix I.(¹)

General lattices

In the general case it is not possible to express the scattering cross section in the vibrational frequency function. We may, however, expand $\mathcal{M}^0_{kk}(t)$ in formula (I.22 a) in powers of t and further proceed exactly as above. The cross section may be written

$$\frac{d^2\sigma_{\text{incoh}}}{d\Omega\, d\omega} = \sum_k \frac{d^2\sigma_k}{d\Omega\, d\omega}, \tag{II.6}$$

where each term on the right side gives the scattering from nuclei with a definite basic index k. For $d^2\sigma_k/d\Omega\, d\omega$ we get

$$\boxed{\frac{d^2\sigma_k}{d\Omega\, d\omega} = A_k \frac{k}{k_0} \frac{(2\pi)^{-\frac{1}{2}}}{\Delta_k} \exp\left[-\frac{(\omega-\omega_0+Q_k)^2}{2\Delta_k^2}\right].} \tag{II.7}$$

Here $$Q_k = \frac{\hbar\varkappa^2}{2M_k}, \qquad \Delta_k^2 = 2Q_k(\mathbf{e}_{\varkappa}\cdot\boldsymbol{\varepsilon}^k\cdot\mathbf{e}_{\varkappa}), \tag{II.8}$$

where $\mathbf{e}_{\varkappa}$ means the unit vector along $\boldsymbol{\varkappa}$ and $\boldsymbol{\varepsilon}^k$ is the (3×3) tensor (²)

$$\varepsilon^k_{xy} = \frac{1}{\hbar N}\sum_s \varepsilon_s C^{k*}_{s,x} C^k_{s,y}. \tag{II.9}$$

$\boldsymbol{\varepsilon}^k$ has the same symmetry as the crystal and therefore for crystals with cubic structure, generally containing several nuclei in each unit cell as, for instance, NaCl, $\boldsymbol{\varepsilon}^k$ is a diagonal tensor with all its diagonal terms equal to

$$\varepsilon^k = \frac{1}{3N\hbar}\sum_s \varepsilon_s |\mathbf{C}^k_s|^2 \tag{II.10}$$

which after multiplication with $\dfrac{3\hbar}{2}$ may be interpreted as the mean kinetic energy of a nucleus with the basic index k.

$\boldsymbol{\varepsilon}^k$ can also be expressed by the components of the dynamical matrix $[\mathcal{D}^{kk'}_{xy}]$ as follows (see ref. [45]).

$$\varepsilon^k_{xy} = \frac{V}{(2\pi)^3}\int_{\text{cell}} \tfrac{1}{2}\,[\mathcal{D}^{\frac{1}{2}} \coth(\beta\mathcal{D}^{\frac{1}{2}})]^{kk}_{xy}\, d\mathbf{q} \tag{II.11}$$

(¹) The proof is based on the harmonic approximation of the interatomic forces, so the "actual momentum distribution" means the distribution obtained in that approximation.

(²) See formula (I.6).

and for $\beta \ll 1$ and $\beta \gg 1$ this expression simplifies to

$$\beta \ll 1; \quad \varepsilon_{xy}^{k} = \frac{1}{2\beta}\left\{\delta_{xy} + \frac{\beta^2}{3}\frac{V}{(2\pi)^3}\int_{\text{cell}} \mathcal{D}_{xy}^{kk}\, d\mathbf{q} - \frac{\beta^4}{45}\frac{V}{(2\pi)^3}\int_{\text{cell}} [\mathcal{D}^2]_{xy}^{kk}\, d\mathbf{q} + \cdots\right\}; \tag{II.11$'$}$$

$$\beta \gg 1: \quad \varepsilon_{xy}^{k} = \frac{V}{(2\pi)^3}\frac{1}{2}\int_{\text{cell}} [\mathcal{D}^{\frac{1}{2}}]_{xy}^{kk}\, d\mathbf{q}. \tag{II.11$''$}$$

From (II.11′) we see that for $\beta \ll 1$ the difference between the scattering from the separate nuclei is mainly due to the mass difference.

Using (I.4) the **q**-integrations in (II.11′) can be performed, giving a direct relation between the scattering and the interatomic force constants.

$$\left.\begin{aligned} \frac{V}{(2\pi)^3}\int_{\text{cell}} \mathcal{D}\, d\mathbf{q} &= \mathcal{V}(0), \\ \frac{V}{(2\pi)^3}\int_{\text{cell}} \mathcal{D}^2\, d\mathbf{q} &= \sum_{\mathbf{R}^l + \mathbf{R}^{l'} = 0} \mathcal{V}(l)\, \mathcal{V}(l'). \end{aligned}\right\} \tag{II.12}$$

$\mathcal{V}(l)$ are then considered as matrixes with the components $\mathcal{V}_{xy}^{kk'}(l)$ and in the latter relation these matrixes are multiplied by each other, for which $\mathbf{R}^l + \mathbf{R}^{l'} = 0$.

The total scattering cross section

Though the total scattering cross section is discussed in a separate part of this paper, some results obtained in the Doppler approximation will be given in this connection. Having first considered a cubic Bravais lattice we can easily generalize the results to other lattices.

The total cross section given in (I.27 a) is first rewritten in the form

$$\sigma_{\text{incoh}} = A\left(\frac{\pi}{\omega_0}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left[-\frac{\omega_0 t^2}{\varrho(t)}\right] \frac{dt}{[\varrho(t)]^{\frac{3}{2}}}, \tag{II.13}$$

where

$$\varrho(t) = -it - \frac{m}{M}[\gamma(t) - \gamma(0)].$$

To get the Doppler scattering we must expand $\gamma(t)$ to the second order in t. After a simple transformation of the integrand we may write

$$\sigma_{\text{incoh}} = A\,\pi^{\frac{1}{2}}\,\lambda^{\frac{3}{2}}\,e^{-\lambda} \lim_{\delta \to 0} \int_{-\infty}^{\infty} \frac{\exp[\mu\lambda^2/(it + \mu\lambda)]}{(it + \mu\lambda)^{\frac{3}{2}}} \frac{dt}{(-it + \delta)^{\frac{1}{2}}} \tag{II.14}$$

with

$$\boxed{\lambda = \frac{3M\hbar\omega_0}{2mE_{\text{kin}}}, \quad \mu = 1 + \frac{m}{M}.} \tag{II.15}$$

δ has been introduced to avoid the singularity at $t=0$, according to the remarks below formula (I.28).

Using the relation (¹)

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ixt}\,\frac{\exp\left[\mu\lambda^2/(it+\mu\lambda)\right]}{(it+\mu\lambda)^{\frac{3}{2}}}\,dt=\begin{cases}\dfrac{1}{\lambda(\mu\pi)^{\frac{1}{2}}}\,e^{-\mu\lambda x}\sinh\left(2\lambda\sqrt{\mu x}\right), & x>0\\ =0 & , \quad x<0\end{cases} \tag{II.16}$$

and Plancherel's theorem for Fourier transforms we now get

$$\sigma_{\text{incoh}}=4A\,\pi^{\frac{1}{2}}\,\mu^{-\frac{1}{2}}\,\lambda^{\frac{1}{2}}\,e^{-\lambda}\int_0^{\infty} x^{\frac{1}{2}}\,e^{-\mu\lambda x}\sinh\left(2\lambda\sqrt{\mu x}\right)dx,$$

and when $x'=x^{\frac{1}{2}}$ has been substituted and a partial integration made, this formula transforms to (²)

$$\boxed{\sigma_{\text{incoh}}=\frac{4\pi A}{\mu^2}\left[\left(1+\frac{1}{2\lambda}\right)\frac{2}{\pi^{\frac{1}{2}}}\,\text{Erf}\,(\lambda^{\frac{1}{2}})+\frac{1}{(\pi\lambda)^{\frac{1}{2}}}\,e^{-\lambda}\right]\cdot} \tag{II.17}$$

For $\lambda \gg 1$ and $\lambda \ll 1$ we may also write

$$\lambda \ll 1:\quad \sigma_{\text{incoh}}=\frac{4\pi A}{\mu^2}\,\frac{2}{\pi^{\frac{1}{2}}}\left(\lambda^{-\frac{1}{2}}+\tfrac{1}{3}\lambda^{\frac{1}{2}}+\cdots\right), \tag{II.17'}$$

$$\lambda \gg 1:\quad \sigma_{\text{incoh}}=\frac{4\pi A}{\mu^2}\left(1+\frac{1}{2\lambda}\right)\cdot \tag{II.17''}$$

Comparing (II.5) and (II.7) we can conclude that the above result may be generalized to general crystals with cubic symmetry in the following way: (³)

$$\sigma_{\text{incoh}}=\sum_k \sigma_k, \tag{II.19}$$

where each σ_k is obtained from (II.17) provided the following substitutions are made:

$$\boxed{A\rightarrow A_k,\qquad \mu\rightarrow 1+\frac{m}{M_k},\qquad \lambda\rightarrow\frac{M_k}{m}\,\frac{\omega_0}{\varepsilon^k}\cdot} \tag{II.19}$$

For non-cubic crystals wo do not obtain such simple results without making further approximations.

(¹) The formula is taken from G. A. Campbell and R. M. Forster, Fourier Integrals, New York 1948.

(²) Erf (x) means the error function.

(³) See the remarks on the tensor $\boldsymbol{\epsilon}^{\mathbf{k}}$ below formula (II.9).

Formula (II.17″) was earlier derived by Placzek [7] and Wick (28] without assuming the harmonic approximation, and they also gave the correction due to the direct binding between the nuclei. Their results may be written in the form

$$\sigma_{\text{incoh}} = \frac{4\pi A}{\mu^2}\left[\underline{1 + \frac{m}{3\,M}\,\frac{E_{\text{kin}}}{\hbar\,\omega_0}} - \frac{m\,\mu^2}{32\,M}\,\frac{C}{(\hbar\,\omega_0)^3} + \cdots\right]. \tag{II.20}$$

C is defined from

$$C = \frac{\hbar^2}{3\,M}\langle(\text{grad}\;V)^2\rangle_T,$$

where V means the potential function for a separate nucleus. In general this formula is valid for $\omega_0 \gg 1$ except for very light nuclei and high temperatures, where the complete expression for the Doppler scattering (II.17) should be used.

Chapter 2. The phonon expansion

Unsymmetric formulation

If the neutron energies and the scattering directions are such that $2\,W$ is of the order of magnitude of unity neither the higher order nor the low order phonon scattering may be neglected. The method to be used must be developed in such a way that significant features of the scattering which depend on the detailed properties of the crystal vibrations are not smoothed out in the approximations used. It is then convenient to take the phonon expansion mentioned before as a starting point for our treatment. The expression for the scattering cross section is first written in a form suitable for direct numerical computation and from which we can also see how to make simplifying approximations. Two different formulations, called the unsymmetric and symmetric ones, are given. Whether the first or the second is most convenient for use depends on the temperature and the scattered neutron energies considered. At first we restrict ourselves to cubic Bravais lattices, making generalization to general lattices in a later chapter.

The phonon expansion is obtained from (II.2) by writing

$$\exp\left(Q\left[\gamma(t) - \gamma(0)\right]\right) = \exp\left[-Q\,\gamma(0)\right]\left[1 + Q\,\gamma(t) + \frac{Q^2}{2}\gamma^2(t) + \cdots\right]$$

and determining the Fourier transform of each power of $\gamma(t)$. Thus the transform of $\gamma(t)/\gamma(0)$

$$g(\omega - \omega_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left[i\,(\omega - \omega_0)\,t\right]\frac{\gamma(t)}{\gamma(0)}\,d\,t \tag{II.21}$$

may be written

$$\boxed{\begin{aligned} g(\omega) &= \frac{f(\omega)}{\omega\gamma(0)}\,\frac{\coth(\beta\omega)-1}{2}, \quad |\omega|\leqslant 1,\\ &= 0 \qquad\qquad\qquad\qquad\quad , \quad |\omega|>1. \end{aligned}} \tag{II.22}$$

$f(\omega)$ is then defined for negative frequencies by

$$f(-\omega)=f(\omega). \tag{II.23}$$

We notice that $g(\omega)$ has the same kind of singularities as $f(\omega)$ and in general shows pronounced maxima and minima(¹), and that $g(\omega)$ is normalized as follows:

$$\int_{-\infty}^{\infty} g(\omega)\,d\omega=1. \tag{II.24}$$

The Fourier transform of any power of $\gamma(t)$ can be expressed in $g(\omega)$. We may write

$$G_n(\omega-\omega_0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\,[i(\omega-\omega_0)\,t]\left[\frac{\gamma(t)}{\gamma(0)}\right]^n dt=$$

$$=\int_{-\infty}^{\infty} g(\omega-\omega_1)\,g(\omega_1-\omega_2)\ldots g(\omega_{n-1}-\omega_0)\,d\omega_1\ldots d\omega_{n-1}.$$

The limit of integration is only formally extended to infinity, for the integrand differs from zero only within a finite interval. We notice that

$$G_n(\omega)=0 \quad \text{for } |\omega|\geqslant n \quad \text{and} \quad \int_{-\infty}^{\infty} G_n(\omega)\,d\omega=1. \tag{II.25}$$

The scattering cross section may now be written in the following form:

$$\boxed{\frac{d^2\sigma_{\text{incoh}}}{d\Omega\,d\omega}=A\,\frac{k}{k_0}\,e^{-2W}\sum_{n=0}^{\infty}\frac{(2W)^n}{n!}\,G_n(\omega-\omega_0).} \tag{II.26}$$

$G_n(\omega)$, which are independent of the scattering direction, are determined from

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(¹) See the frequency functions given by Walker [31] and Squires [23] for Al and by Jakobsen [32] for Cu.

$$\left.\begin{aligned} G_0(\omega) &= \delta(\omega), \\ G_1(\omega) &= g(\omega), \\ G_2(\omega) &= \int_{-\infty}^{\infty} g(\omega-\omega')\, G_1(\omega')\, d\omega', \\ &\dots\dots\dots\dots\dots \\ G_{n+1}(\omega) &= \int_{-\infty}^{\infty} g(\omega-\omega')\, G_n(\omega')\, d\omega'. \end{aligned}\right\} \qquad \text{(II.27)}$$

This formulation is unsymmetric in as far as $G_n(-\omega) \neq G_n(\omega)$. For high temperatures the asymmetry is small but at the absolute zero $G_n(\omega) = 0$ for $\omega > 0$, owing to the fact that phonon absorption is then impossible.

The first term in (II.26) corresponds to pure elastic scattering and the intensity depends on the crystal vibrations only by the Debye-Waller factor. The second term is very simply related to the vibrational frequency function and, as especially emphasized by Placzek and Van Hove [22], this fact can be used to determine the frequency function experimentally by measuring the energy spectrum of the neutrons scattered in a certain direction. Such experiments have recently been performed with fairly good results [15, 17–18]. The higher phonon terms are then depressed by using cold neutrons.

The multi-phonon terms are, however, much less sensitive to detailed assumptions regarding the crystal vibrations and it would therefore be possible to perform fairly accurate calculations of these terms without detailed information about the crystal properties. The Debye model would certainly be accurate enough for most purposes but it does not greatly reduce the numerical work. In the next chapter we will therefore use another method, which has been applied in mathematical statistics to calculate Faltung-integrals as appearing in (II.27).

For $2W \ll 1$ the phonon expansion converges rapidly but for larger values of $2W$ the convergence is slow and a method of summing up the main part of the phonon terms will be given.

Symmetric formulation

When (II.26) is used for direct numerical computation it is often more convenient to transform this expression as follows to get a more symmetric form. We write

$$g(\omega) = e^{-\beta\omega} \underbrace{\frac{f(\omega)}{2\,\omega\,\gamma(0)\,\sinh(\beta\omega)}}_{\bar{g}(\omega)}$$

and transform (II.26) to

$$\boxed{\frac{d^2\sigma_{\text{incoh}}}{d\Omega\, d\omega} = A\,\frac{k}{k_0}\, e^{-2W-\beta(\omega-\omega_0)} \sum_{n=0}^{\infty} \frac{(2W)^n}{n!}\, \bar{G}_n(\omega-\omega_0).} \qquad \text{(II.28)}$$

$\bar{G}_n(\omega)$ is determined analogous to (II.27).

$$\left.\begin{aligned}\bar{G}_0(\omega) &= \delta(\omega),\\ \bar{G}_1(\omega) &= \bar{g}(\omega) = \frac{f(\omega)}{2\,\omega\,\gamma(0)\sinh(\beta\,\omega)}, \quad |\omega| \leqslant 1,\\ &= 0, \quad |\omega| > 1,\\ &\dots\dots\dots\dots\dots\\ \bar{G}_{n+1}(\omega) &= \int_{-\infty}^{\infty} \bar{g}(\omega-\omega_1)\,\bar{G}_n(\omega_1)\,d\,\omega_1.\end{aligned}\right\} \tag{II.29}$$

In that case $\bar{G}_n(-\omega) = \bar{G}_n(\omega)$. The whole asymmetry appears in the factor $\exp[-\beta(\omega-\omega_0)]$.(1)

Especially for high temperatures, when the asymmetry is small, and further if we wish to determine the intensity of neutrons that have gained energy in the scattering it seems more convenient to base approximations on (II.28) rather than on (II.26).

The Debye approximation

As mentioned before the Debye model for the crystal vibrations is certainly a good approximation for the higher phonon terms, and for high temperatures further approximations can be made, after which $\bar{G}_n$ can be easily calculated. $\bar{g}(\omega)$ is expanded in powers of β.

$$\bar{g}(\omega) = \frac{3}{2\beta\gamma(0)}\left(1-\frac{\beta^2}{6}\omega^2+\cdots\right), \quad |\omega| \leqslant 1 \tag{II.30}$$

and for $\beta \ll 1$ we may thus approximate to

$$\left.\begin{aligned}\bar{g}(\omega) &= \frac{1}{2}, \quad |\omega| \leqslant 1,\\ &= 0, \quad |\omega| > 1.\end{aligned}\right\} \tag{II.31}$$

$\gamma(0)$ has then in an analogous way been approximated

$$\gamma(0) = \frac{3}{\beta} = \frac{6\,T}{\Theta}, \quad \Theta = \text{Debye temperature},$$

If we now write $\bar{G}_n(\omega)$ in the following form, which corresponds to the approximation in (II.31),

$$\bar{G}_n(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}\left(\frac{\sin t}{t}\right)^n d\,t, \tag{II.32}$$

the integration is easily performed by calculus of residue. We get the following result:

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(1) Note that $\bar{G}_n(\omega)$ is not normalized to unity as $G_n(\omega)$.

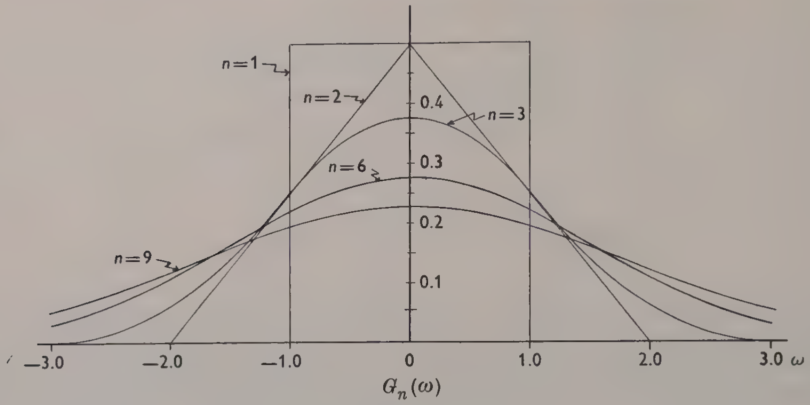

Fig. 1.

$$\boxed{\begin{aligned}\bar{G}_n(\omega) &= n\,2^{-n}\sum_{\nu=0}^{[(n-|\omega|)/2]}(-1)^{\nu}\frac{(n-2\nu-|\omega|)^{n-1}}{\nu!\,(n-\nu)!}, && |\omega|\leqslant n,\\ &=0, && |\omega|>n.\end{aligned}} \tag{II.33}$$

The summation is extended over all integers from zero to the largest one below $(n-|\omega|)/2$.

We notice that in this approximation $\bar{G}_n(\omega)$ are independent of the temperature. The figure above (Fig. 1), where some of the $\bar{G}_n$ are drawn, shows the functions for $n>2$ to be very similar to Gaussian ones. This fact will be used in the next chapter to calculate the high-phonon scattering cross sections for general lattices.

Chapter 3. Expansion of $G_n(\omega)$ in Hermite polynomials

Unsymmetric formulation

It is a well-known fact that $G_n(\omega)$ always tends to a Gaussian function as n increases.(¹) The same is of course also valid for $\bar{G}_n(\omega)$, as illustrated in Fig. 1.

To account for the deviation from a Gaussian function $G_n(\omega)$ is expanded into Hermite orthogonal functions as shown in the following. The method is described in textbooks on mathematical statistics and therefore a brief summary is sufficient in the present context.(²) Owing to the fact that $G_n(\omega)$ is different from zero only within a finite interval we have no trouble with the convergence of the expansion. The essential thing is, however, that even in very accurate calculations we need not consider more than the first few terms in the expansion and for more approximate calculations all but the first term may be neglected.(³)

(¹) This theorem is known as "The central limit theorem". See for instance: H. Cramér, Mathematical methods of statistics, Uppsala 1945, p. 213.

(²) See for instance: H. Cramér, loc. cit. p. 185, 221. See also: C. G. Essén, Acta Math., 77, 1 (1944).

(³) We only treat G_n for $n\geqslant 2$ in this approximate way.

To get a convenient starting point for our treatment $G_n(\omega)$ is written in the following form (see the foregoing chapter):

$$G_n(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \left[\frac{\gamma(t)}{\gamma(0)}\right]^n dt. \tag{II.34}$$

We further notice that $$|\gamma(t)| < |\gamma(0)| \quad \text{for } t \neq 0, \tag{II.35}$$

except for an ideal Einstein crystal, where $\gamma(t)$ is strictly periodic in t, and that

$$\gamma(t) = o(t^{-1}) \quad \text{when } t \to \infty. \tag{II.35$'$}$$

The latter property is due to the fact that the vibrational frequency function is continuous and its derivative is integrable.(¹) For large values of n a small region around $t=0$ makes the main contribution to the integral except possibly for large values on ω, where, however, the function is very small. $\gamma(t)$ is therefore expanded in powers of t. We may write as follows:

$$\frac{\gamma(t)}{\gamma(0)} = \sum_{\nu=0}^{\infty} \frac{\alpha_\nu}{\nu!} (i t)^\nu, \tag{II.36}$$

where the coefficients α_ν are determined from the vibrational frequency function by the following relations

$$\left.\begin{aligned}
&\alpha_0 = 1, && \alpha_1 = \frac{1}{\gamma(0)}; \\
&\alpha_2 = \frac{1}{\gamma(0)} \int_0^1 \zeta \coth(\beta\zeta) f(\zeta)\, d\zeta = \frac{4\, E_{\text{kin}}}{3\hbar\,\gamma(0)}, && \alpha_3 = \frac{1}{\gamma(0)} \int_0^1 \zeta^2 f(\zeta)\, d\zeta; \\
&\alpha_4 = \frac{1}{\gamma(0)} \int_0^1 \zeta^3 \coth(\beta\zeta) f(\zeta)\, d\zeta && \cdots\cdots\cdots\cdots
\end{aligned}\right\} \tag{II.36}$$

The corresponding expansion for $\ln[\gamma(t)/\gamma(0)]$ is written

$$\ln\left[\frac{\gamma(t)}{\gamma(0)}\right] = \sum_{\nu=0}^{\infty} \frac{\varkappa_\nu}{\nu!} (i t)^\nu, \tag{II.37}$$

and $\varkappa_\nu$ are then determined from the α_ν by

$$\left.\begin{aligned}
&\varkappa_1 = \alpha_1, \\
&\varkappa_2 = \alpha_2 - \alpha_1^2, \\
&\varkappa_3 = \alpha_3 - 3\alpha_1\alpha_2 + 2\alpha_1^2, \\
&\varkappa_4 = \alpha_4 - 3\alpha_2^2 - 4\alpha_1\alpha_3 + 12\alpha_1^2\alpha_2 - 6\alpha_1^4 \\
&\cdots\cdots\cdots\cdots\cdots\cdots
\end{aligned}\right\} \tag{II.37$'$}$$

(¹) Van Hove [9] has shown on rather general assumptions that $\gamma(t) = 0(t^{-\frac{3}{2}})$. For an ideal Debye crystal the frequency function is discontinuous and in that case $\gamma(t) = 0(t^{-1})$.

For convenience we introduce a special notation Δ_0^2 for $\varkappa_2$ and this is thus defined by

$$\boxed{\Delta_0 = \left[\frac{4E_{\text{kin}}}{3\hbar\gamma(0)} - \frac{1}{[\gamma(0)]^2}\right]^{\frac{1}{2}}.} \tag{II.38}$$

$G_n(\omega)$ can now be treated as follows:

$$G_n = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}\exp\left[n\ln\left(\frac{\gamma(t)}{\gamma(0)}\right)\right]dt =$$

$$= \frac{1}{2\pi\Delta_0\sqrt{n}}\int_{-\infty}^{\infty}\exp\left(-\frac{t^2}{2}+i\frac{\omega+\frac{n}{\gamma(0)}}{\Delta_0\sqrt{n}}t\right)\exp\left[n\sum_{\nu=3}^{\infty}\frac{\varkappa_\nu}{\nu!}\left(\frac{it}{\Delta_0\sqrt{n}}\right)^{\nu}\right]dt =$$

$$= \frac{1}{2\pi\Delta_0\sqrt{n}}\sum_{\nu=0}^{\infty}c_\nu^{(n)}\int_{-\infty}^{\infty}(-it)^{\nu}\exp\left(-\frac{t^2}{2}+i\frac{x_n}{\Delta_0\sqrt{n}}t\right)dt =$$

$$= \frac{1}{\Delta_0\sqrt{2\pi n}}\exp\left(-x_n^2/2n\Delta_0^2\right)\sum_{\nu=0}^{\infty}(-1)^{\nu}c_\nu^{(n)}H_\nu\left(x_n/\Delta_0\sqrt{n}\right).$$

x_n denotes $\omega + n/\gamma(0)$. $H_\nu(x)$ are the Hermite polynomials.(¹) The first few included in the series above are given explicitly below.

$$\left.\begin{aligned}
H_0(x) &= 1,\\
H_3(x) &= x^3 - 3x,\\
H_4(x) &= x^4 - 6x^2 + 3,\\
H_6(x) &= x^6 - 15x^4 + 45x^2 - 15.
\end{aligned}\right\} \tag{II.39}$$

The $c_\nu^{(n)}$ coefficients are determined from

(¹) The Hermite polynomials are defined in agreement with the definition used by Cramér (loc. cit.) and also found in Jahnke–Emde, Funktionentafeln, Leipzig und Berlin 1938; thus

$$e^{-x^2/2}H_n(x) = (-1)^n\frac{d^n}{dx^n}\left(e^{-x^2/2}\right).$$

Tables of $(2\pi)^{-\frac{1}{2}}\frac{d^n}{dx^n}\left(e^{-x^2/2}\right)$ may be found e.g. in Cramér's book, p. 557.

$$\left.\begin{aligned}
&c_0^{(n)}=1, \quad c_1^{(n)}=c_2^{(n)}=0,\\
&c_3^{(n)}=\frac{\varkappa_3}{3\,!\,\Delta_0^3}\,\frac{1}{n^{\frac{1}{2}}}=\frac{\gamma_1}{n^{\frac{1}{2}}},\\
&c_4^{(n)}=\frac{\varkappa_4}{4\,!\,\Delta_0^4}\,\frac{1}{n}=\frac{\gamma_2}{n},\\
&c_5^{(n)}=\frac{\varkappa_5}{5\,!\,\Delta_0^5}\,\frac{1}{n^{\frac{3}{2}}},\\
&c_6^{(n)}=\frac{\varkappa_6}{6\,!\,\Delta_0^6}\,\frac{1}{n^2}+\frac{\varkappa_3^2}{(3\,!\Delta_0^3)^2}\,\frac{1}{2\,n},\\
&\cdots\cdots\cdots\cdots
\end{aligned}\right\}\qquad \text{(II.40)}$$

The symbols γ_1 and γ_2 are introduced to get a shorter notation. They depend on the temperature and the frequency function and can be tabulated provided the latter is known.

If the terms in the expansion above are arranged in powers of $n^{-\frac{1}{2}}$ we get the following expression for $G_n(\omega)$ including only the first three terms:

$$\boxed{\begin{aligned}G_n(\omega)=\frac{1}{\Delta_0\sqrt{2\pi n}}\exp\left(-x_n^2/2\,n\,\Delta_0^2\right)\Big\{1-\frac{\gamma_1}{\sqrt{n}}\,H_3(x_n/\Delta_0\sqrt{n})+\\
+\frac{1}{n}\left[\gamma_2\,H_4(x_n/\Delta_0\sqrt{n})+\tfrac{1}{2}\,\gamma_1^2\,H_6(x_n/\Delta_0\sqrt{n})\right]\Big\}.\end{aligned}}\qquad \text{(II.41)}$$

As already mentioned x_n is given by $x_n=\omega+n/\gamma(0)$.

The first term in (II.41) will in all applications give the main part of the scattering and in many cases we may neglect all other terms. Owing to this fact it might in almost all cases be sufficient to use the Debye approximation when computing γ_1 and γ_2 as long as one keeps in mind that uncertainties in $\gamma(0)$ and Δ_0 will have quite a great effect on the Gaussian function. In that case γ_1 and γ_2 depend only on β and may be tabulated once and for all. Tables of them are found in Appendix II.

It may, however, be essential to have more exact values on $\gamma(0)$ and Δ_0 and in calculating these more realistic assumptions on the frequency function should then be made. For $\beta \ll 1$ and for $\beta \gg 1$ we may write as follows, if $\langle\omega^n\rangle$ denotes

$$\langle\omega^n\rangle=\int_0^1\omega^n\,f(\omega)\,d\omega: \qquad \text{(II.42)}$$

$$\left.\begin{aligned}
\gamma(0)&=\frac{\langle\omega^{-2}\rangle}{\beta}+\frac{\beta}{3}-\frac{\beta^3}{45}\langle\omega^2\rangle+\cdots, \quad \beta\ll 1,\\
&=\langle\omega^{-1}\rangle, \qquad\qquad \beta\gg 1,\\
[\gamma(0)\,\Delta_0]^2&=\frac{\langle\omega^{-2}\rangle}{\beta^2}+\frac{1}{3}\left(\langle\omega^{-2}\rangle\langle\omega^2\rangle-2\right)+\frac{\beta^2}{45}\left(4\langle\omega^2\rangle-\langle\omega^{-2}\rangle\langle\omega^4\rangle\right)+\cdots,\ \beta\ll 1,\\
&=\left(\langle\omega^{-1}\rangle\langle\omega\rangle-1\right), \quad \beta\gg 1.
\end{aligned}\right\}$$

(II.43)

From this expression we conclude that especially for high temperatures it is possible to use the Debye approximation also in determining $\gamma(0)$ and Δ_0 provided that the Debye temperature is conveniently defined. To get good values of both $\gamma(0)$ and Δ_0 we define the Debye temperature as follows:

$$\Theta = \frac{\hbar\,\omega_D}{k_B} = \frac{\hbar\sqrt{3}}{k_B\langle\omega^{-2}\rangle^{\frac{1}{2}}}. \tag{II.44}$$

In chapter 1, however, we saw that for high neutron energies $\gamma(0)$ disappears from the expression for the scattering cross section. Our results will thus be quite insensitive to the values adopted for $\gamma(0)$, provided that the same value is used in the Debye–Waller factor. In that energy region it would therefore be more accurate to define Θ as follows, giving a more precise value for Δ_0.

$$\Theta = \frac{\hbar\sqrt{5}\,\langle\omega^2\rangle^{\frac{1}{2}}}{k_B\sqrt{3}}. \tag{II.45}$$

Tables of $\gamma(0)$ and Δ_0 obtained in the Debye approximation are given in Appendix II.

In a later chapter the approximation (II.41) will be compared with exact results obtained from (II.27) by direct numerical integration, assuming a certain form of the vibrational frequency function.

Let us, however, first return to the first term, the Gaussian term, in our expansion above and show how to sum over n to get an expression which is more convenient for the calculation of the main part of the two- and higher phonon scattering.

The Gaussian term

We would have obtained the Gaussian term without corrections if we had in (II.27) simply changed $g(\omega)$ to

$$g_1(\omega) = \frac{1}{\Delta_0(2\pi)^{\frac{1}{2}}}\exp\left[-\left(\omega+\frac{1}{\gamma(0)}\right)^2 \Big/ 2\,\Delta_0^2\right]. \tag{II.46}$$

The actual function $g(\omega)$ is then approximated by a Gaussian function with the same mean value and the same spread as the original function.

$$\langle\omega\rangle = \int_{-\infty}^{\infty}\omega\,g(\omega)\,d\omega = -\frac{1}{\gamma(0)}, \qquad \langle(\omega-\langle\omega\rangle)^2\rangle = \int_{-\infty}^{\infty}(\omega-\langle\omega\rangle)^2\,g(\omega)\,d\omega = \Delta_0^2,$$

and the two functions are further normalized in the same way.

$$\int_{-\infty}^{\infty} g(\omega)\,d\omega = \int_{-\infty}^{\infty} g_1(\omega)\,d\omega = 1.$$

If the Gaussian terms are inserted into (II.26) the sum over n may be transformed as follows:

$$\sum_{n=2}^{\infty} \frac{(2W)^n}{n!} \frac{1}{\Delta_0 (2\pi n)^{\frac{1}{2}}} \exp\left[-\frac{(\omega-\omega_0+n/\gamma(0))^2}{2n\Delta_0^2}\right] = \frac{1}{\Delta_0} e^{-\beta_1 x} \sum_{n=2}^{\infty} \frac{z^n}{n!} \frac{\exp(-x^2/2n)}{(2\pi n)^{\frac{1}{2}}}.$$

z, x and β_1, respectively, are defined by

$$\boxed{z=Q\gamma(0)\exp(-\tfrac{1}{2}\beta_1^2), \qquad x=\frac{1}{\Delta_0}(\omega-\omega_0), \qquad \beta_1=\frac{1}{\Delta_0\gamma(0)}.} \tag{II.47}$$

These quantities depend on the temperature since $\gamma(0)$ and Δ_0 depend on temperature. The above sum defines a function $F(z, x)$ which is evidently independent of the structure of the crystal and may thus be tabulated once and for all. In appendix II this function is given for a series of values of z and x.

$$F(z, x)=\sum_{n=2}^{\infty} \frac{z^n}{n!} \frac{\exp(-x^2/2n)}{(2\pi n)^{\frac{1}{2}}}. \tag{II.48}$$

The scattering cross section may now be written in the following form:

$$\boxed{\frac{d^2\sigma_{\text{incoh}}}{d\Omega\, d\omega}=A\frac{k}{k_0}e^{-Q\gamma(0)}\left[\delta(\omega-\omega_0)+Q\gamma(0)g(\omega-\omega_0)+\frac{1}{\Delta_0}e^{-\beta_1 x}F(z, x)+F_{\text{corr}}\right].} \tag{II.49}$$

F_{corr} denotes the correction due to all but the first term in the expansion (II.41). Where only an approximate calculation is required we may neglect this correction term.

In such approximate calculations we may also for temperatures higher than the Debye temperature make further simplifications as follows:

$$\gamma(0)=\frac{6T}{\Theta}, \qquad \Delta_0=\frac{1}{\sqrt{3}}, \qquad \beta_1=\frac{\Theta\sqrt{3}}{6T}. \tag{II.50}$$

In determining z we may put $\beta_1=0$.

It will finally be proved that for large $Q\gamma(0)$ the Gaussian approximation correctly gives the Doppler scattering earlier discussed. To show this the Gaussian terms are written in the form

$$\frac{1}{\Delta_0(2\pi n)^{\frac{1}{2}}}\exp(-x_n^2/2n\Delta_0^2)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(i x_n t-\tfrac{1}{2}n\Delta_0^2 t^2)\,dt$$

and subsequently inserted into the formula (II.26). Owing to the fact that the one-phonon scattering decreases rapidly for increasing values of the Debye-Waller function we may also treat this term in the Gaussian approximation without appreciable error for the whole scattering cross section. We then write as follows.

$$\sum_{n=0}^{\infty}\frac{(2W)^n}{n!}G_n(\omega-\omega_0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[i(\omega-\omega_0)t\right]\left\{\sum_{n=0}^{\infty}\frac{1}{n!}\left[Q\gamma(0)\exp\left(\frac{it}{\gamma(0)}-\frac{1}{2}\Delta_0^2t^2\right)\right]^n\right\}=$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[i(\omega-\omega_0)t\right]\exp\left[Q\gamma(0)\exp\left(\frac{it}{\gamma(0)}-\frac{1}{2}\Delta_0^2t^2\right)\right]dt.$$

If we now proceed in the same way as in chapter 1, expanding

$$\exp\left(\frac{it}{\gamma(0)}-\frac{1}{2}\Delta_0^2t^2\right)=1+i\frac{t}{\gamma(0)}-\frac{1}{2}\left(\Delta_0^2+\frac{1}{[\gamma(0)]^2}\right)t^2+\cdots$$

we get the following result after the integration over t:

$$\sum_{n=0}^{\infty}\frac{(2W)^n}{n!}G_n(\omega-\omega_0)=\frac{1}{\Delta(2\pi)^{\frac{1}{2}}}e^{2W}\exp\left[-(\omega-\omega_0+Q)^2/2\Delta^2\right). \qquad \text{(II.51)}$$

Δ is then the same quantity as defined in (II.5′) and the formula above corresponds exactly to that in (II.5). We see how the factor e^{2W} cancels the Debye-Waller factor and how the quantity $\gamma(0)$, being essential for low energies, disappears in that case.

Symmetric formulation

As mentioned before it is, where possible, more convenient to base the approximate treatment on the symmetric formula (II.28) and we will therefore discuss this case as well. We may proceed in exactly the same way as above and need thus only give a very brief presentation emphasizing the modifications to be made.

$\bar{g}(\omega)$ is first written in the form

$$\bar{g}(\omega)=\frac{\bar{\gamma}(0)}{\gamma(0)}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\omega t}\left[\frac{\bar{\gamma}(t)}{\bar{\gamma}(0)}\right]dt, \qquad \text{(II.52)}$$

where
$$\bar{\gamma}(t)=\int_{0}^{1}\frac{f(\zeta)}{\zeta\sinh(\beta\zeta)}\cos(\zeta t)\,d\zeta. \qquad \text{(II.52′)}$$

Analogous to (II.34) we have

$$\bar{G}_n(\omega)=\left[\frac{\bar{\gamma}(0)}{\gamma(0)}\right]^n\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\omega t}\left[\frac{\bar{\gamma}(t)}{\bar{\gamma}(0)}\right]^n dt. \qquad \text{(II.53)}$$

$\gamma(t)$ is further expanded in powers of t.

$$\frac{\bar{\gamma}(t)}{\bar{\gamma}(0)}=\sum_{\nu=0}^{\infty}\frac{\bar{\alpha}_\nu}{\nu!}(it)^\nu,$$

where all odd coefficients $\bar{\alpha}_1, \bar{\alpha}_3, \ldots$ now vanish and the even ones are determined from

$$\left.\begin{aligned} &\bar{\alpha}_0 = 1, && \bar{\alpha}_2 = \frac{1}{\bar{\gamma}(0)} \int_0^1 \frac{\zeta f(\zeta)}{\sinh(\beta\zeta)} d\zeta, \\ &\bar{\alpha}_4 = \frac{1}{\bar{\gamma}(0)} \int_0^1 \frac{\zeta^3 f(\zeta)}{\sinh(\beta\zeta)} d\zeta, && \ldots\ldots\ldots\ldots \end{aligned}\right\} \tag{II.54}$$

The coefficients corresponding to $\varkappa_\nu$ are determined from (II.37′) with $\bar{\alpha}_\nu$ inserted instead of the α_ν. The quantity $\bar{\Delta}_0$, corresponding to Δ_0, is in that case defined as follows:

$$\boxed{\bar{\Delta}_0^2 = \bar{\alpha}_2 = \frac{1}{\bar{\gamma}(0)} \int_0^1 \frac{\zeta f(\zeta)}{\sinh(\beta\zeta)} d\zeta.} \tag{II.55}$$

The expansion of $\bar{G}_n(\omega)$ in the Hermite polynomials may be written as

$$\bar{G}_n(\omega) = \left[\frac{\bar{\gamma}(0)}{\gamma(0)}\right]^n \frac{1}{\bar{\Delta}_0 (2\pi n)^{\frac{1}{2}}} \exp(-\omega^2/2n\bar{\Delta}_0^2) \sum_{\nu=0}^{\infty} (-1)^\nu \bar{c}_\nu^{(n)} H_\nu(\omega/\bar{\Delta}_0 \sqrt{n}). \tag{II.56}$$

This formula is simpler than the corresponding unsymmetric one in two respects. Firstly only $\bar{c}_\nu^{(n)}$ with even ν are nonvanishing and secondly x_n, introduced earlier, is in this case independent of n. The even $\bar{c}_\nu^{(n)}$ are given by

$$\left.\begin{aligned} &\bar{c}_0^{(n)} = 1, \quad \bar{c}_2^{(n)} = 0, \\ &\bar{c}_4^{(n)} = \frac{\bar{\alpha}_4 - 3\bar{\alpha}_2^2}{4!\,\bar{\Delta}_0^4} \frac{1}{n} = \frac{\bar{\gamma}_2}{n}, \end{aligned}\right\} \tag{II.57}$$

and the formula corresponding to (II.41) takes the form

$$\bar{G}_n(\omega) = \left[\frac{\bar{\gamma}(0)}{\gamma(0)}\right]^n \frac{1}{\bar{\Delta}_0 (2\pi n)^{\frac{1}{2}}} \exp(-\omega^2/2n\bar{\Delta}_0^2) \left[1 + \frac{\bar{\gamma}_2}{n} H_4(\omega/\bar{\Delta}_0 \sqrt{n})\right]. \tag{II.58}$$

Inserting this expression for $\bar{G}_n(\omega)$ into (II.28) the scattering cross section may be written in the following form:

$$\boxed{\begin{aligned} \frac{d^2\sigma_{\text{incoh}}}{d\Omega\, d\omega} = A \frac{k}{k_0} \exp[-Q\gamma(0) - \beta(\omega-\omega_0)] \Big\{ &\delta(\omega-\omega_0) + Q\gamma(0)\bar{g}(\omega-\omega_0) + \\ &+ \frac{1}{\bar{\Delta}_0} F(z_1, x_1) + \frac{\bar{\gamma}_2}{\bar{\Delta}_0} F_1(z_1, x_1) \Big\}. \end{aligned}} \tag{II.59}$$

z_1 and x_1 are defined by

$$z_1 = Q\bar{\gamma}(0), \qquad x_1 = (\omega-\omega_0)/\bar{\Delta}_0 \tag{II.60}$$

and $F(z, x)$ is the function introduced in (II.48). $F_1(z, x)$ is defined in an analogous way by

$$F_1(z,x)=\sum_{n=2}^{\infty}\frac{z^n}{n!\,n}\,\frac{\exp\left(-x^2/2n\right)}{(2\pi n)^{\frac{1}{2}}}\,H_4(x/\sqrt{n}) \tag{II.61}$$

and refers to the second term in (II.58).

It must be noted that the formula (II.59) cannot in general be used for low temperatures. For in that case the unsymmetric factor $\exp\left(-\beta(\omega-\omega_0)\right)$ has such an effect that $\exp\left(-\beta(\omega-\omega_0)\right)[\ldots]$ has its maximum value for an ω outside the region of validity of (II.58). The formula should therefore mainly be used for rather high temperatures. It is immediately seen that (II.59) and (II.49) are then approximately equal. The factor $\exp\left(-\beta_1 x\right)$, for instance, tends to $\exp\left(-\beta(\omega-\omega_0)\right)$ as the temperature increases. It may also be shown that the Gaussian approximation does not exactly give the Doppler scattering for $2W \gg 1$ but only an approximate expression valid for temperatures that are not too low.

General lattices

The same method as above may be used to derive approximate expressions for the scattering cross section for general lattices. We must then, however, start from the general formula (I.22 a) and make the expansion

$$\exp\left(\boldsymbol{\varkappa}\cdot\mathcal{M}^0_{kk}\cdot\boldsymbol{\varkappa}\right)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\boldsymbol{\varkappa}\cdot\mathcal{M}^0_{kk}\cdot\boldsymbol{\varkappa}\right)^n.$$

Subsequently $(\mathbf{e}_\varkappa\cdot\mathcal{M}^0_{kk}(t)\cdot\mathbf{e}_\varkappa)/(\mathbf{e}_\varkappa\cdot\mathcal{M}^0_{kk}(0)\cdot\mathbf{e}_\varkappa)$ is expanded in powers of t in the same way as earlier for $\gamma(t)/\gamma(0)$. $\mathbf{e}_\varkappa$ denotes the unit vector along $\boldsymbol{\varkappa}$. The treatment is the same as for simple cubic crystals and therefore we will give the results only, restricting ourselves to the unsymmetric formulation, which has a larger range of validity. We can, however, easily derive an expression analogous to (II.58). Moreover the modification mainly consists of exchanging coth $(\ldots)$ for $1/\sinh(\ldots)$ in the symmetrical formulation and putting all odd coefficients α^k_ν below equal to zero.

In the unsymmetric formulation we get the following expression for the α^k_ν, which correspond to the earlier coefficients α_ν and here refer to a certain basic index k.

$$\left.\begin{aligned}
&\alpha^k_0=1,\quad \alpha^k_1=\frac{1}{\gamma_k(0)},\\
&\alpha^k_2=\frac{1}{\gamma_k(0)}\frac{1}{N}\sum_s\omega_s\coth(\beta\omega_s)\,|\mathbf{e}_\varkappa\cdot\mathbf{C}^k_s|^2=\frac{2}{\gamma_k(0)}\,(\mathbf{e}_\varkappa\cdot\boldsymbol{\varepsilon}^k\cdot\mathbf{e}_\varkappa),^{(1)}\\
&\alpha^k_3=\frac{1}{\gamma_k(0)}\frac{1}{N}\sum_s\omega^2_s\,|\mathbf{e}_\varkappa\cdot\mathbf{C}^k_s|^2,\\
&\alpha^k_4=\frac{1}{\gamma_k(0)}\frac{1}{N}\sum_s\omega^3_s\coth(\beta\omega_s)\,|\mathbf{e}_\varkappa\cdot\mathbf{C}^k_s|^2,\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots
\end{aligned}\right\}\tag{II.62}$$

---

(1) $\boldsymbol{\varepsilon}^k$ was defined in (II.9).

$\gamma_k(0)$ is that part of the Debye–Waller function $2W_k$ which is dependent on temperature and is defined as follows:

$$\gamma_k(0) = \frac{1}{N} \sum_s \omega_s^{-1} \coth(\beta\omega_s) \, |\mathbf{e}_\varkappa \cdot \mathbf{C}_s^k|^2. \tag{II.63}$$

With these notations and the ones corresponding to x_n, Δ_0, γ_1 and γ_2 we may write the scattering cross section in the following form:

$$\boxed{\begin{aligned} \frac{d^2\sigma_{\text{incoh}}}{d\Omega\, d\omega} &= \sum_k \frac{d^2\sigma_{\text{incoh}}^{(k)}}{d\Omega\, d\omega}, \\ \frac{d^2\sigma_{\text{incoh}}^{(k)}}{d\Omega\, d\omega} &= A_k \frac{k}{k_0} \exp(-2W_k) \sum_{n=0}^{\infty} \frac{(2W_k)^n}{n!} G_n^{(k)}. \end{aligned}}$$

$G_0^{(k)}$ and $G_1^{(k)}$ are defined by (¹)

$$\left.\begin{aligned} G_0^{(k)} &= \delta(\omega - \omega_0) \\ G_1^{(k)} &= \frac{1}{\gamma_k(0)} \frac{1}{N} \sum_{s,\varepsilon} \frac{\coth(\beta\omega_s) + \varepsilon}{2\omega_s} |\mathbf{e}_\varkappa \cdot \mathbf{C}_s^k|^2 \, \delta(\omega - \omega_0 + \varepsilon\omega_s) \end{aligned}\right\} \tag{II.65}$$

and $G_n^{(k)}$ are for $n \geqslant 2$ approximately given by

$$\begin{aligned} G_n^{(k)} = \frac{1}{\Delta_{0,k}(2\pi n)^{\frac{1}{2}}} \exp(-x_n^2/2n\Delta_{0,k}^2) \Big[1 - \frac{\gamma_{1,k}}{n} H_3(x_n/\Delta_{0,k}\sqrt{n}) + \\ + \frac{1}{n} \{\gamma_{2,k} H_4(x_n/\Delta_{0,k}\sqrt{n}) + \tfrac{1}{2}\gamma_{1,k}^2 H_6(x_n/\Delta_{0,k}\sqrt{n})\} \Big]. \end{aligned} \tag{II.66}$$

Analogous to the earlier notation x_n is defined by

$$x_n = \omega - \omega_0 + \frac{n}{\gamma_k(0)}. \tag{II.67}$$

Chapter 4. Numerical comparisons

In order to gauge the accuracy of the approximations discussed in the last chapter some numerical calculations have been made assuming a certain form of the vibrational frequency function. In the first case (II.31) was supposed exactly valid, where formula (II.33) could be used to determine $G_n(\omega)$ precisely. These were also calculated from the approximate formula (II.41), referred to as Approx. A, and in the Gaussian approximation, where the scattering constants $\gamma(0)$, Δ_0, γ_1 and γ_2 were determined in agreement with the adopted frequency distribution. This case corresponds fairly well to a Debye-like crystal in the case of high temperatures.

(¹) $\int_{-\infty}^{\infty} G_n^{(k)} \, d\omega = 1$ only if $\mathbf{e}_\varkappa$ is held fix.

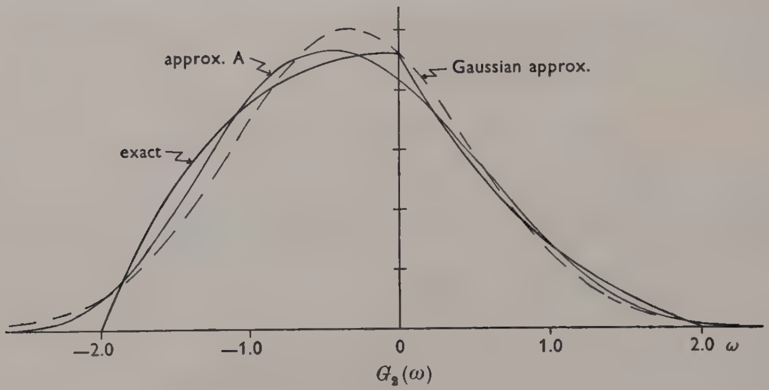

Fig. 2.

In the next two cases we consider a realistic frequency function far from a Debye distribution, supposing in one case room temperature and in the other a rather low temperature. The vibrational frequency distribution adopted is that which Walker [31] obtained for Al from measurements on diffuse X-ray diffraction.(¹) The calculations were performed exactly by using formula (II.27) (²) and further in Approx. A and in the Gaussian approximation. The scattering constants were determined in accordance with the adopted frequency function, and thus the discrepancies between the different calculations are due only to the truncation of the expansion in Hermite functions.

Case I

According to (II.31) $g(\omega)$ is supposed to be equal to

$$\left.\begin{aligned} g(\omega) &= \frac{\beta}{2\sinh\beta}e^{-\beta\omega}, \quad &|\omega|<1,\\ &=0, &|\omega|>1. \end{aligned}\right\} \tag{II.68}$$

$g(\omega)$ is then correctly normalized. The corresponding expression for $\gamma(t)$ is

$$\gamma(t)=\frac{3}{\beta}\,\frac{\sinh(\beta+it)}{\beta+it}, \tag{II.69}$$

and from this we easily obtain the coefficients α_ν. The calculation was made for $\beta=0.5$, and the scattering constants then have the following values:

$$\frac{1}{\gamma(0)}=0.164, \quad \Delta_0=0.563, \quad \gamma_1=-0.058, \quad \gamma_2=-0.043.$$

The results of the different computations are presented in Figs. 2–3.

(¹) Walker's frequency distribution is adopted only to have a realistic frequency spectrum for the numerical calculations.

(²) The exact calculations were performed on the electronic computer "Besk" in Stockholm. The author is very grateful to Miss G. Hambraeus and Mr. T. Berggren for valuable help in making a program for these calculations.

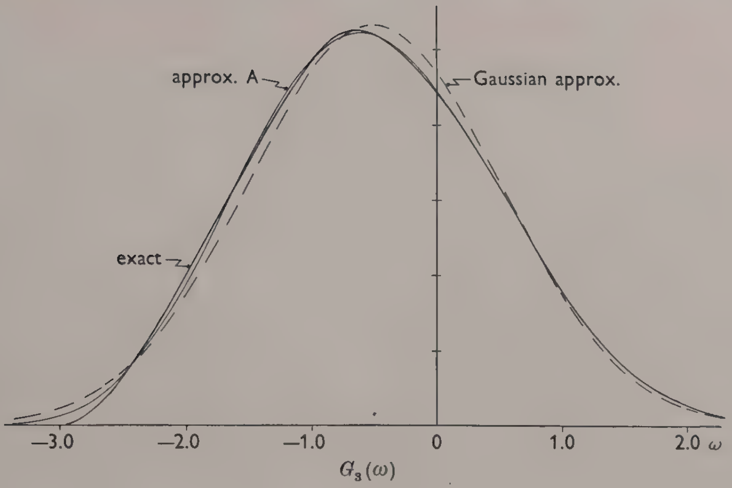

Fig. 3.

Case II.

$\beta = 0.748$ corresponds to the supposed temperature $T = 300°K$ and to the maximum vibrational frequency $\omega_m = 5.91 \times 10^{13}$ sec^{-1}. The scattering constants have the values

$$\frac{1}{\gamma(0)} = 0.163, \quad \Delta_0 = 0.457, \quad \gamma_1 = -0.062, \quad \gamma_2 = -0.037.$$

$f(\omega)/\omega^2$ and $g(\omega)$ are shown in the first two figures (Figs. 4–5) and Figs. 6–8 present the numerical results for G_2, G_3 and G_4. G_2 is also calculated assuming the ideal Debye frequency distribution and making the computations according to the exact formula (II.27). The Debye frequency ω_D is defined so as to give the correct value for $Q\gamma(0)$ as follows:

$$\gamma(0) = \gamma_D(0)/\omega_D, \tag{II.70}$$

where $\gamma_D(0)$ is taken from the table in Appendix II for $\beta_D = \hbar\,\omega_D/2\,k_B T = 0.748\,\omega_D$. From this definition we get $\omega_D = 0.83$ ($\beta_D = 0.62$). The values for the scattering constants above, obtained in the Debye approximation, are (¹)

$$\Delta_0 = 0.455, \quad \gamma_1 = -0.071, \quad \gamma_2 = -0.038.$$

We see that these agree surprisingly well with the exact ones.

Case III

In this case we assume $\beta = 3.00$ ($T = 74.8°$K) and the corresponding values for the scattering constants are

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(¹) As Δ_0 depends on the unit in which the frequencies are measured we must relate Δ_D and Δ_0 as follows:

$$(\omega - \omega_0)/\omega_m\,\Delta_0 = (\omega - \omega_0)/\omega_D\,\Delta_D,$$

where Δ_D is obtained from the tables in Appendix II for $\beta_D = 0.62$. γ_1 and γ_2 on the contrary do not depend on the units used.

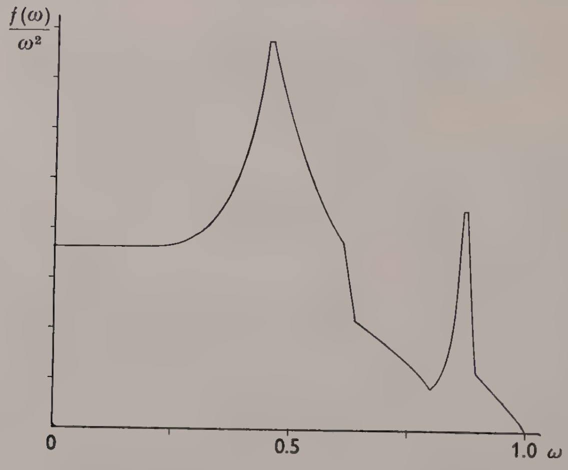


Fig. 4.

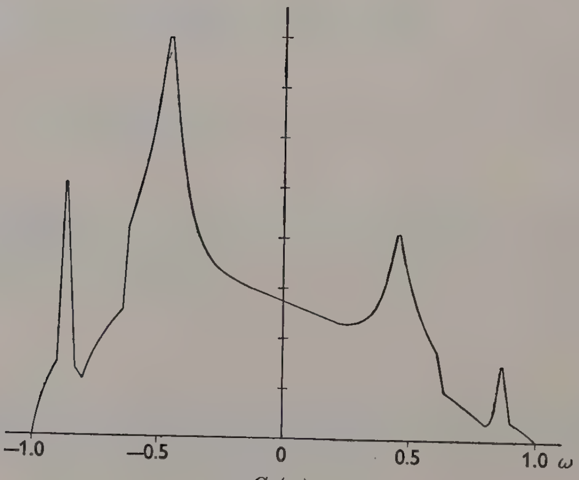


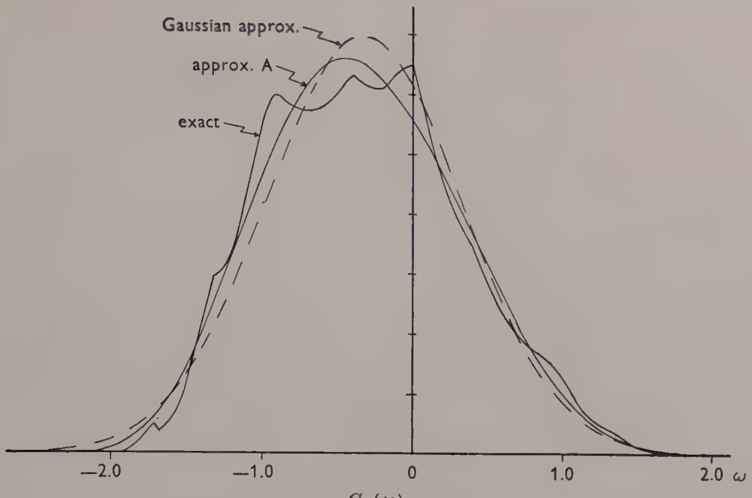
Fig. 5.

$$\frac{1}{\gamma(0)}=0.432, \quad \Delta_0=0.320, \quad \gamma_1=-0.140, \quad \gamma_2=0.034.$$

If defining the Debye frequency as in the preceding case we get in the Debye approximation ($\omega_D=0.836$, $\beta_D=2.50$).

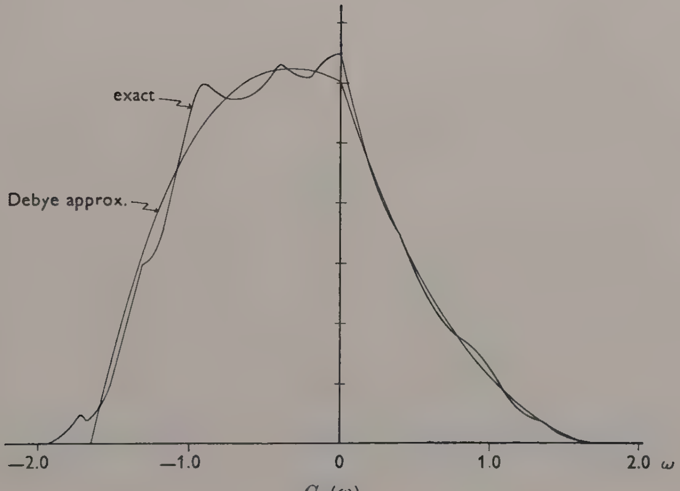
$$\Delta_0=0.314, \quad \gamma_1=-0.171, \quad \gamma_2=0.030.$$

$g(\omega)$ is drawn in Fig. 9 and Figs. 10–12 show G_2, G_3 and G_4 respectively.



$G_2(\omega)$

Fig. 6 a.



$G_2(\omega)$

Fig. 6 b.

Some conclusions may be drawn from these numerical comparisons. Thus the approximation given in (II.41) seems to give very accurate values except for the two-phonon term. The more simple Gaussian approximation also fits fairly well and should be accurate enough in many applications. To obtain the two-

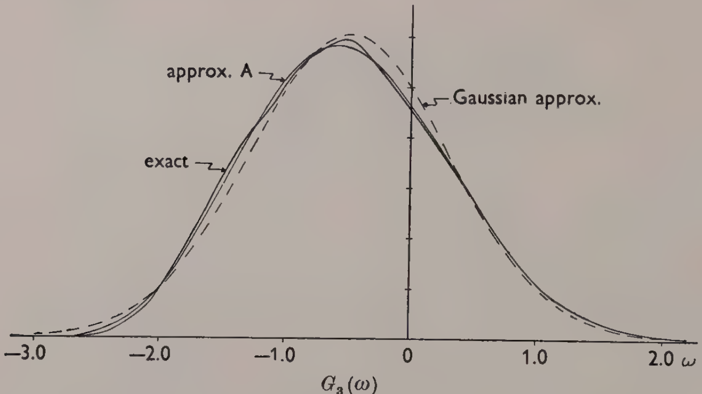


Fig. 7.

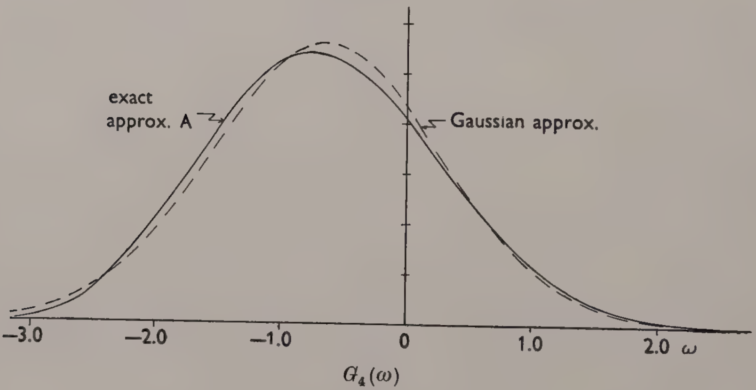


Fig. 8.

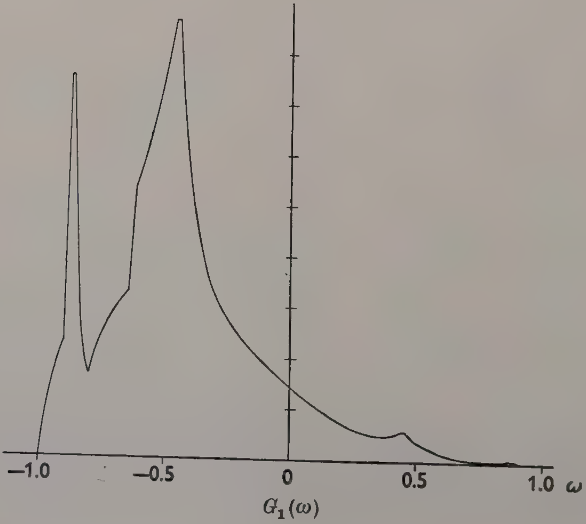


Fig. 9.

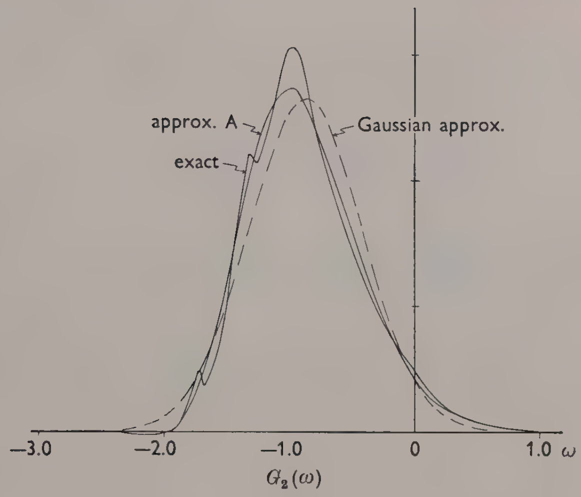


Fig. 10.

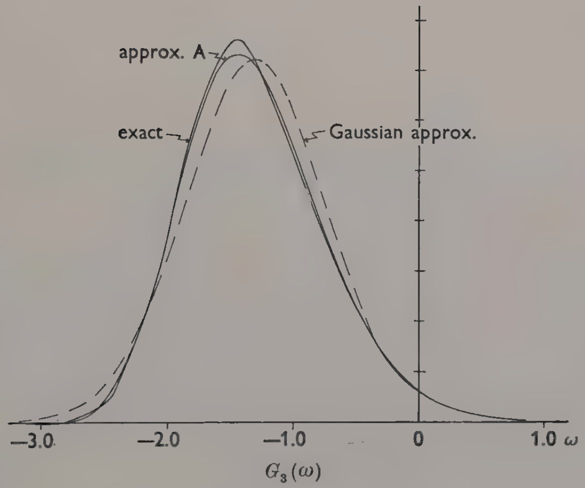


Fig. 11.

phonon term more accurately we must use a realistic frequency function and the exact formula (II.27), which moreover in that case is nearly as simple as the other expressions given. The use of a Debye frequency distribution does not seem to give much better results than our other approximations.

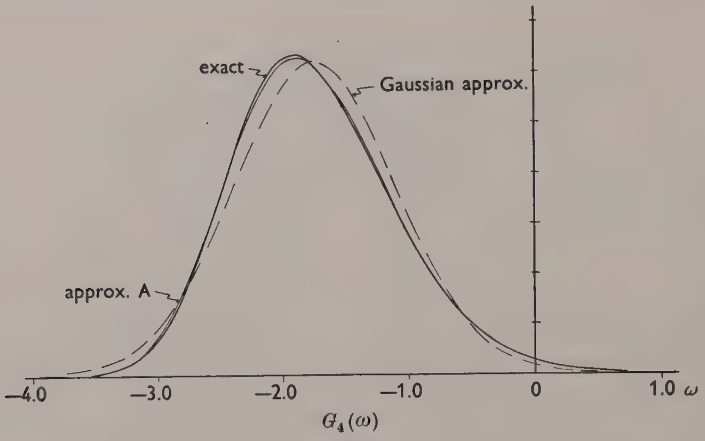


Fig. 12.

PART III

TOTAL SCATTERING CROSS SECTION

Chapter 1. Expansion of the total scattering cross section in powers of m/M

General formulation

As already mentioned the total cross section can be brought into a convenient form for direct numerical calculations if it is expanded in powers of m/M. Except for very light nuclei and high temperatures this series converges rapidly and in general only two or three terms need be considered. Placzek restricts himself to a Debye crystal (¹) and in this chapter some of his results will therefore be generalized to real crystals to get an idea of how the details of the vibrational properties manifest themselves in the total cross section. In order not to complicate the mathematical treatment we specialize to cubic Bravais lattices, where all effects of the lattice vibrations are determined by the frequency function. We can, however, easily modify the results to make them valid for general crystals.

An expression for the incoherent total cross section was given in (II.13) and after introducing a function $\Phi(t)$, defined by

$$\varrho(t) = (-it)(1+\Phi), \qquad \Phi = \frac{m}{M}\frac{\gamma(t)-\gamma(0)}{it}, \tag{III.1}$$

the cross section can be rewritten as follows:

(¹) For large neutron energies, however, Placzek gives results valid under more general conditions [7].

$$\sigma_{\text{incoh}} = A \left(\frac{\pi}{\omega_0}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} (-i\,t)^{-\frac{3}{2}} \exp\,(-i\,\omega_0 t)\, F(t)\, d\,t, \tag{III.2}$$

where

$$F(t) = (1+\Phi)^{-\frac{3}{2}} \exp\left(i\,\omega_0\, t \frac{\Phi}{1+\Phi}\right). \tag{III.3}$$

As Φ is proportional to m/M, the m/M expansion is obtained by simply expanding $F(t)$ in powers of Φ and making the integration term by term. If $|\Phi| < 1$ everywhere, corresponding to the condition

$$\frac{m}{M}\gamma(0) \lesssim 1 \quad \left(\text{or } \frac{m}{M}\frac{6\,T}{\Theta} \lesssim 1,\ \ \Theta = \text{the Debye temperature}\right), \tag{III.4}$$

the series converges for arbitrary neutron energies $\hbar\,\omega_0$.

We thus write

$$F(t) = 1 + (i\,\omega_0\, t - \tfrac{3}{2})\,\Phi + \cdots.$$

The final integration is easily performed if it is noted that

$$\begin{aligned} \lim_{\delta\to 0} \int_{-\infty}^{\infty} (-i\,t+\delta)^{-(n+\frac{3}{2})}\, e^{-ixt}\, d\,t &= \frac{2^{n+2}\,\pi^{\frac{1}{2}}\, x^{n+\frac{1}{2}}}{1.3.5\,\ldots\,(2\,n+1)}, \qquad x>0, \\ &= 0, \qquad\qquad\qquad\qquad\quad x<0, \end{aligned} \tag{III.5}$$

and the total cross section may be put in the following form

$$\boxed{\sigma_{\text{incoh}} = 4\,\pi\, A \sum_{n=0}^{\infty} \left(\frac{m}{M}\right)^{n} \sigma_n,} \tag{III.6}$$

where the first two σ_n are given by (1)

$$\left.\begin{aligned} &\sigma_0 = 1, \\ &\sigma_1 = \omega_0 \int_{\operatorname{Max}(-\omega_0,\,-1)}^{1} \frac{f(\omega)}{\omega}\,[\coth\,(\beta\,\omega) - 1] \left(1+\frac{\omega}{\omega_0}\right)^{\frac{1}{2}} \left(1+\frac{\omega}{2\,\omega_0}\right) d\,\omega - 2\,\omega_0\,\gamma(0). \end{aligned}\right\} \tag{III.7}$$

Large and small neutron energies

A more convenient form for numerical calculations is obtained by further expanding (III.7) in powers of $1/\omega_0$ $(\omega_0 > 1)$. The treatment is straightforward and the result for σ_1 can be written in the form

---

(1) Cf.: D. A. Kleinman, Thesis, Brown University, 1951.

$$\boxed{\sigma_1 = \sum_{n=0}^{\infty} \frac{c_n'}{\omega_0^n} \int_{-1}^{1} \omega^n f(\omega) [\coth(\beta\omega) - 1] \, d\omega,} \tag{III.8}$$

where the coefficients $c_n' = \frac{1}{2}\left(\frac{3}{n+1} - 1\right)\binom{\frac{1}{2}}{n}$. (1)

$$c_0' = 1, \quad c_1' = \tfrac{1}{8} \quad c_2' = 0, \quad c_3' = -\tfrac{1}{128}, \quad c_4' = \tfrac{1}{128}, \quad c_5' = -\tfrac{7}{1024}.$$

A corresponding formula is obtained for $\omega_0 < 1$ by expanding in powers of $\omega_0^{\frac{1}{2}}$. We then get

$$\boxed{\sigma_1 = \frac{c_0''}{\omega_0^{\frac{1}{2}}} + c_1'' \omega_0^{\frac{1}{2}} + c_2'' \omega_0 + c_3'' \omega_0^{\frac{3}{2}} + \cdots} \tag{III.9}$$

$$\left.\begin{aligned} c_0'' &= \frac{1}{2} \int_0^1 \omega^{\frac{1}{2}} f(\omega) [\coth(\beta\omega) - 1] \, d\omega, \\ c_1'' &= \frac{5}{4} \int_0^1 \omega^{-\frac{1}{2}} f(\omega) [\coth(\beta\omega) - 1] \, d\omega, \\ c_2'' &= -2 \int_0^1 \omega^{-1} f(\omega) \coth(\beta\omega) \, d\omega, \\ c_3'' &= \tfrac{7}{16} \int_0^1 \omega^{-\frac{3}{2}} f(\omega) [\coth(\beta\omega) - 1] \, d\omega, \end{aligned}\right\} \tag{III.9'}$$

The linear term in ω_0 comes from the elastic part of the scattering.

The Debye approximation

If Debye's approximation for the vibrational frequency distribution is used, a simplified expression for σ_1 is obtained also by making an expansion in powers of β ($\beta = \hbar/2\,k_B T = \Theta/2\,T$). We then get a formula which may be used for arbitrary neutron energies. We write

$$\left.\begin{aligned} \coth(\beta\omega) &= \frac{1}{\beta\omega} + \frac{\beta\omega}{3} - \frac{(\beta\omega)^3}{45} + \cdots, \\ \gamma(0) &= \frac{3}{\beta} + \frac{\beta}{3} - \frac{\beta^3}{75} + \cdots. \end{aligned}\right\} \tag{III.10}$$

The ω-integration is now easily performed and gives

---

(1) $\binom{m}{n}$ are the binomial coefficients.

$$\boxed{\sigma_1 = \frac{Q_0(\omega_0)}{\beta} + Q_1(\omega_0) + \beta\, Q_2(\omega_0) + 0(\beta^3).} \tag{III.11}$$

$Q_n(\omega_0)$ are determined from

$$\left.\begin{aligned} Q_0(\omega_0) &= \omega_0 \left[\left(1+\frac{1}{\omega_0}\right)^{\frac{3}{2}} f_0(1+\omega_0) + \left(1-\frac{1}{\omega_0}\right)^{\frac{3}{2}} f_0(1-\omega_0) - 6\right], \\ Q_1(\omega_0) &= \omega_0 \left[\left(1+\frac{1}{\omega_0}\right)^{\frac{3}{2}} f_1(1+\omega_0) - \left(1-\frac{1}{\omega_0}\right)^{\frac{3}{2}} f_1(1-\omega_0)\right], \\ Q_2(\omega_0) &= \tfrac{1}{3}\,\omega_0 \left[\left(1+\frac{1}{\omega_0}\right)^{\frac{3}{2}} f_2(1+\omega_0) + \left(1-\frac{1}{\omega_0}\right)^{\frac{3}{2}} f_2(1-\omega_0) - 2\right], \end{aligned}\right\} \tag{III.11'}$$

where

$$\left.\begin{aligned} f_0(x) &= \tfrac{8}{5}x - 1 \\ f_1(x) &= \tfrac{4}{7}x^2 - 2x + 1, \\ f_2(x) &= \tfrac{32}{105}x^3 - \tfrac{48}{35}x^2 + \tfrac{12}{5}x - 1. \end{aligned}\right\} \tag{III.11''}$$

For $\omega_0 < 1$ the terms $(1-1/\omega_0)^{\frac{3}{2}} f_n(1-\omega_0)$ should be omitted.

Higher order terms

To derive expressions for the higher order terms in the m/M-expansion it would be easier to start from formula (II.26) (¹) and expand the differential scattering cross section in powers of m/M before making the integration over the frequencies of the scattered neutrons.(²) The integration over the scattering angles leads to a set of functions

$$\Phi_n(x) = (1+x)^{2n+2} - (1-x)^{2n+2} \tag{III.12}$$

and after the integration over ω we get the following expression:

$$\boxed{\sigma_{\text{incoh}} = 4\pi A \sum_{n=0}^{\infty} \left[\frac{m}{M}\gamma(0)\right]^n \bar{\sigma}_n.} \tag{III.13}$$

$$\left.\begin{aligned} \bar{\sigma}_0 &= 1. \\ \bar{\sigma}_1 &= \frac{1}{8}\omega_0 \left[\int_0^\infty \Phi_1\left(\sqrt{\frac{\omega}{\omega_0}}\right) G_1(\omega-\omega_0)\, d\omega - 16\right], \\ \bar{\sigma}_2 &= \frac{1}{12}\,\omega_0^2 \left[\int_0^\infty \Phi_2\left(\sqrt{\frac{\omega}{\omega_0}}\right) \{\tfrac{1}{2} G_2(\omega-\omega_0) - G_1(\omega-\omega_0)\}\, d\omega + 32\right], \\ \bar{\sigma}_3 &= \frac{1}{16}\,\omega_0^3 \left[\int_0^\infty \Phi_3\left(\sqrt{\frac{\omega}{\omega_0}}\right) \{\tfrac{1}{6} G_3(\omega-\omega_0) - \tfrac{1}{2} G_2(\omega-\omega_0) + \tfrac{1}{2} G_1(\omega-\omega_0)\}\, d\omega - \tfrac{128}{3}\right]. \end{aligned}\right\} \tag{III.13'}$$

(¹) To get an idea of the convergence of the series it was, however, convenient to base the derivation on formula (II.13) as done above.

(²) Cf.: G. Placzek, Phys. Rev., *105*, 1240 (1957).

For large neutron energies ($\omega_0 > 1$) a modification of the m/M expansion can be made, as shown by Wick [28], so that the first term in the series gives the high energy limit with the exact mass correction, $4\pi A/(1+m/M)^2$. We can easily derive this expansion from (II.13) by expanding the integrand in powers of $(1+m/M)\,t/\omega_0$ and then integrate term by term. This series represents an asymptotic expansion in $1/\omega_0$ and the first three terms are found in (II.20).

Chapter 2. Phonon expansion

General formulation

As found in the last chapter the use of the m/M-expansion is restricted to cases where the factor $(m/M)\,\gamma(0)$ is not too large. In order to derive approximate formulae that do not have such restrictions on their applicability we will discuss the total cross section also from another point of view. We then specialize to very slow neutrons, a case of great interest, and base the treatment on the phonon expansion and the approximation (II.58) for the separate phonon terms.(1) In some respects our results will thus complete those obtained from the m/M expansion. As (II.58) gives a good approximation for two and higher phonon terms only, the total scattering cross sections from zero- and one-phonon scattering should be calculated separately, using more accurate approximations.

To get the total cross section from (II.28) we must first make an integration over the scattering angles, which, when expanding in powers of ω_0, leads to the following expression (2):

$$\int (2\,W)^n\, e^{-2W}\, d\Omega = 4\pi \left[\frac{m}{M}\gamma(0)\right]^n \exp\left[-\frac{m}{M}\gamma(0)\,\omega\right]\left\{\omega^n + \omega_0\left[\frac{2\,n^2+n}{3}\,\omega^{n-1} - \frac{4\,n+3}{3}\,\frac{m}{M}\gamma(0)\,\omega^n + \frac{2}{3}\left[\frac{m}{M}\gamma(0)\right]^2 \omega^{n+1}\right] + \cdots\right\}. \tag{III.14}$$

$\bar{G}_n(\omega-\omega_0)$, taken from (II.58), is also expanded in powers of ω_0, accounting only for the zero-order and the linear term in ω_0, and the final integration over ω then leads to Weber–Hermite functions as follows: (3)

$$\int_0^\infty \omega^{n+\frac{1}{2}} \exp\left(-a\,\omega - \frac{\omega^2}{2\,n\,\bar{\Delta}_0^2}\right) d\,\omega = (\bar{\Delta}_0\sqrt{n})^{n+\frac{3}{2}}\,\Gamma\left(n+\tfrac{3}{2}\right) e^{n x^2/4}\, D_{-(n+\frac{3}{2})}(x\sqrt{n})\,. \tag{III.15}$$

a and x are related to the vibrational properties of the crystal by

$$a = \frac{m}{M}\gamma(0) + \beta, \qquad x = \left(\frac{m}{M}\gamma(0)+\beta\right)\bar{\Delta}_0\,. \tag{III.16}$$

---

(1) Note that for small values of ω_0 and not too low temperatures ($\beta\omega_0 \lesssim 1$) approximation (II.58) is more accurate than (II.41) and in addition gives expressions more simple to handle.

(2) We have $2\,W = (m/M)\,\gamma(0)\,(\omega + \omega_0 - 2\sqrt{\omega\,\omega_0}\cos\vartheta)$ where ϑ is the scattering angle.

(3) See for instance: Erdelyi, Magnus, Oberhettinger, and Tricomi, Higher Transcendental Functions, vol. 2, pp. 116–130, New York 1953.

The contribution to the total cross section by the nth order term in the phonon expansion is written in the following form (cf. formulae (III.6) and (III.9):

$$\sigma_{\mathrm{incoh}}^{(n)}=\frac{4\pi A}{\omega_0^{\frac{1}{2}}}\left[\sigma_1^{(n)}+\omega_0\,\sigma_2^{(n)}+\cdots\right]. \tag{III.17}$$

The term $\sigma_1^{(n)}$ is further divided into two parts $\sigma_{1,0}^{(n)}$ and $\sigma_{1,1}^{(n)}$ where the first part refers to the Gaussian approximation in (II.58) and the second part to the correction term. In (III.17) the linear term in ω_0 should be considered as a rather small correction and $\sigma_2^{(n)}$ is therefore determined only in the Gaussian approximation. The three parts are explicitly given below and our task is to put them into at form convenient for numerical calculations.

$$\sigma_{1,0}^{(n)}=\frac{\bar{\Delta}_0^{\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}}\,\frac{(\sqrt{n})^{n+\frac{1}{2}}\,\Gamma\left(n+\frac{3}{2}\right)}{\Gamma(n+1)}\left[\frac{m}{M}\bar{\gamma}(0)\,\bar{\Delta}_0\right]^n e^{nx^2/4}\,D_{-(n+\frac{3}{2})}(x\sqrt{n})\,; \tag{III.18}$$

$$\begin{aligned}\sigma_{1,1}^{(n)}=\frac{\bar{\Delta}_0^{\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}}\,\frac{(\sqrt{n})^{n+\frac{1}{2}}\,\Gamma\left(n+\frac{3}{2}\right)}{n\,\Gamma(n+1)}\left[\frac{m}{M}\bar{\gamma}(0)\,\bar{\Delta}_0\right]^n e^{nx^2/4}\,\bar{\gamma}_2\Bigg\{\Bigg[n^2x^4+&\\ +\left(3n^2+\frac{3n}{2}\right)x^2+\left(n^2-n-\frac{3}{4}\right)\Bigg]\,D_{-(n+\frac{3}{2})}(x\sqrt{n})-&\\ -x\sqrt{n}\,(n\,x^2+2\,n)\,D_{-(n+\frac{1}{2})}(x\sqrt{n})\,;&\end{aligned} \tag{III.18'}$$

$$\begin{aligned}\sigma_2^{(n)}=\frac{\bar{\Delta}_0^{-\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}}\,\frac{(\sqrt{n})^{n+\frac{1}{2}}\,\Gamma\left(n+\frac{3}{2}\right)}{\Gamma(n+1)}\left[\frac{m}{M}\bar{\gamma}(0)\,\bar{\Delta}_0\right]^n e^{nx^2/4}\Bigg\{\Bigg[\frac{2}{3}x^2-\frac{4}{3}\beta\,\bar{\Delta}_0\,x+&\\ +\left(\frac{2}{3}+\frac{1}{n}+\frac{2}{3}\beta^2\,\bar{\Delta}_0^2\right)\Bigg]\sqrt{n}\,D_{-(n+\frac{1}{2})}(x\sqrt{n})-\Bigg[\frac{2\,n}{3}x^3-\frac{4\,n}{3}\beta\,\bar{\Delta}_0\,x^2+&\\ +x\left(2+\frac{4\,n}{3}+\frac{2\,n}{3}\beta^2\,\bar{\Delta}_0^2\right)-\left(\frac{4\,n}{3}+2\right)\beta\,\bar{\Delta}_0\Bigg]\,D_{-(n+\frac{3}{2})}(x\sqrt{n})\Bigg\}\cdot&\end{aligned} \tag{III.18''}$$

The derivation of the formulae (III.18) is rather lengthy but elementary. The relation

$$\left(n+\frac{3}{2}\right)D_{-(n+\frac{5}{2})}(z)=D_{-(n+\frac{1}{2})}(z)-z\,D_{-(n+\frac{3}{2})}(z) \tag{III.19}$$

between the Weber–Hermite functions has been used to express the cross section in only two of them and $(m/M)\,\gamma(0)\,\bar{\Delta}_0$ has been exchanged for $(x-\beta\,\bar{\Delta}_0)$. Finally the terms are suitably rearranged.

Approximate formula for $\sigma_{1,0}^{(n)}$

In further simplifying the expression for $\sigma_{1,0}^{(n)}$ the approximate expression for $D_{(n+\frac{3}{2})}(x\sqrt{n})$ derived in Appendix III, is inserted into (III.18) and the proportionality factor depending on n, which then appears, is approximated as follows:

$$\frac{\sqrt{n}\,\Gamma\left(n+\frac{1}{2}\right)}{\Gamma(n+1)}=1-\frac{1}{8n}+\cdots. \tag{III.20}$$

The terms are finally arranged in powers of $1/n$ and we then get the following expression for $\sigma_{1,0}^{(n)}$:

$$\boxed{\sigma_{1,0}^{(n)}=\frac{\Delta_0^{\frac{1}{2}}}{2\pi^{\frac{1}{2}}}\,\frac{\left(1+\frac{1}{4}x^2\right)^{\frac{1}{2}}-\frac{1}{2}x}{\left(1+\frac{1}{4}x^2\right)^{\frac{1}{4}}}\,z^n\left[1+\frac{1}{n}h_1(x)+\cdots\right]}\,. \tag{III.21}$$

x and z depend on the vibrations of the crystal according to

$$\begin{aligned} x&=\left(\frac{m}{M}\gamma(0)+\beta\right)\bar{\Delta}_0, \\ z&=\frac{m}{M}\bar{\gamma}(0)\bar{\Delta}_0\left(\sqrt{1+\frac{x^2}{4}}-\frac{x}{2}\right)\exp\left[\frac{1}{2}\left(\sqrt{1+\frac{x^2}{4}}-\frac{x}{2}\right)^2\right] \end{aligned} \tag{III.22}$$

and $h_1(x)$ is defined by

$$h_1(x)=\frac{1}{8}\,\frac{x\left[\left(1+\frac{1}{4}x^2\right)^{\frac{1}{2}}+\frac{1}{2}x\right]}{1+\frac{1}{4}x^2}-\frac{1}{8}+\varphi_1(x). \tag{III.23}$$

$\varphi_1(x)$ is given in Appendix III. The contribution by this term is only a few per cent and may in general be neglected.

To get an idea of the validity of the approximations made in the derivation we will consider the two special cases $x=0$ and $x=\infty$ in more detail. In these cases (III.15) is easily integrated exactly and a comparison with the approximate values obtained from (III.21) can be made.

$x=0$: The exact and the approximate expressions differ only by the following proportionality factor

$$\frac{\text{approx. value}}{\text{exact value}}=\frac{\Gamma(n+1)\,e^{n/2}}{\left(\sqrt{2n}\right)^{n+\frac{1}{2}}\Gamma\left(\frac{1}{2}n+\frac{3}{4}\right)}\left(1-\frac{5}{48n}\right) \tag{III.24}$$

which is given numerically in Table 1 for some values of n.

Table 1.

n	1	2	3	4
ratio	0.966	0.992	0.996	0.998

$x=\infty$: In this case the two formulae differ by the following factor

$$\frac{\text{approx. value}}{\text{exact value}} = \frac{\sqrt{n}\,\Gamma(n+1)}{\Gamma(n+\frac{3}{2})}\left(1+\frac{3}{8n}\right), \tag{III.25}$$

and the numerical values are given in Table 2.

Table 2.

n	1	2	3	4
ratio	1.035	1.011	1.005	1.002

Approximate formula for $\sigma_{1,1}^{(n)}$

The expression for $\sigma_{1,1}^{(n)}$ in (III.18′) has been approximated in essentially the same way as $\sigma_{1,0}^{(n)}$. The derivation is more complicated, however. To get a consistent approximation for all values of x the $1/n^2$ term in the asymptotic expansion of the Weber–Hermite functions must also be considered (see Appendix III). To simplify the final expression some terms that are small for all values of x have been neglected. The result may be written in the following form:

$$\boxed{\sigma_{1,1}^{(n)} = \frac{\Delta_0^{\frac{1}{2}}}{2\pi^{\frac{1}{2}}}\,\frac{(1+\frac{1}{4}x^2)^{\frac{1}{2}}-\frac{1}{2}x}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}}\,z^n\,\bar{\gamma}_2\left[n\,g_1(x)+g_2(x)+\frac{1}{n}\,g_3(x)+\cdots\right]\cdot} \tag{III.26}$$

The functions g_1, g_2 and g_3 are given below.

$$g_1(x) = \left(\sqrt{1+\frac{x^2}{4}}-\frac{x}{2}\right)^4,$$

$$g_2(x) = \left(\frac{3}{2}-\frac{5}{2}\,\frac{1}{1+\frac{1}{4}x^2}\right)\left(\sqrt{1+\frac{x^2}{4}}-\frac{x}{2}\right)^2-\frac{15}{8}\,\frac{x}{1+\frac{1}{4}x^2}\left(\sqrt{1+\frac{x^2}{4}}-\frac{x}{2}\right),$$

$$\begin{aligned} g_3(x) = {} & -\frac{3}{4}+\frac{1}{16}\left(\sqrt{1+\frac{x^2}{4}}+\frac{x}{2}\right)\left[(3x^3-2x)\left(1+\frac{x^2}{4}\right)^{-1}-\frac{3}{2}(x^4+3x^2+1)\cdot\right. \\ & \left.\cdot\left(1+\frac{x^2}{4}\right)^{-\frac{3}{2}}+\frac{5}{2}(x^4+3x^2+1)\left(1+\frac{x^2}{4}\right)^{-\frac{5}{2}}\right] \\ = {} & -\frac{11}{16}-\frac{3x}{32}+\frac{9x^2}{128}+\cdots, \quad x \ll 1, \\ = {} & 3-27x^{-2}+\cdots, \quad x \gg 1. \end{aligned}$$

We notice that as x increases ($\beta \to 0$) and the high phonon terms contribute more and more to the cross section both g_1 and g_2 tend to zero. Owing to this fact the Gaussian approximation will be more accurate for small values of β. Such phonon terms as are not at all approximated by the Gaussian approximation (very large values of n) do not contribute appreciably.

Approximate formula for $\sigma_2^{(n)}$

The derivation is made as for $\sigma_{1,0}^{(n)}$, so we only write the final result.

$$\boxed{\sigma_2^{(n)} = \frac{1}{\bar{\Delta}_0} \frac{\bar{\Delta}_0^{\frac{1}{2}}}{2\pi^{\frac{1}{2}}} \frac{(1+\frac{1}{4}x^2)^{\frac{1}{2}} - \frac{1}{2}x}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}} z^n \left[n\,p_1(x) + p_2(x) + \frac{1}{n} p_3(x) + \cdots \right],} \qquad \text{(III.30)}$$

where

$$p_1(x) = \frac{2}{3}\left(\sqrt{1+\frac{x^2}{4}} - \frac{x}{2}\right)^3 + \beta\bar{\Delta}_0 \frac{4}{3}\left(\sqrt{1+\frac{x^2}{4}} - \frac{x}{2}\right)^2 + \beta^2\bar{\Delta}_0^2 \frac{2}{3}\left(\sqrt{1+\frac{x^2}{4}} - \frac{x}{2}\right),$$

$$p_2(x) = \left(\frac{4}{3} - \frac{4x}{3} + \frac{x^2}{3} + \cdots\right) + \beta\bar{\Delta}_0\left(2 - \frac{x}{2} - \frac{x^2}{4} + \cdots\right) + \beta^2\bar{\Delta}_0^2\left(\frac{1}{3} + \frac{x}{6} - \frac{3x^2}{8} + \cdots\right), \; x \ll 1$$

$$= \left(-\frac{2}{3}x^{-1} + \frac{18}{3}x^{-3} + \cdots\right) + \beta\bar{\Delta}_0(6x^{-2} - 22x^{-4} + \cdots) + \beta^2\bar{\Delta}_0^2\left(\frac{4}{3}x^{-1} + 4x^{-3}\right), \; x \gg 1$$

$$p_3(x) = \left(\frac{1}{2} - \frac{x}{12} - \frac{x^2}{3} + \cdots\right) + \beta\bar{\Delta}_0\left(\frac{1}{12} + \frac{x}{3} + \frac{x^4}{48} + \cdots\right) - \beta^2\bar{\Delta}_0^2\left(\frac{x^2}{24} + \cdots\right), \; x \ll 1$$

$$= (-8x^{-2} + \cdots) + \beta\bar{\Delta}_0(23x^{-2} + \cdots) - \beta^2\bar{\Delta}_0^2\left(-\frac{1}{2}x^{-1} + \cdots\right), \; x \gg 1$$

p_2 and p_3 are given only for small and large values of x.

Summation over the phonon terms

The summation over the phonon terms is now easily made. Including the one-phonon term we get the following expression for the inelastic cross section (cf. formulae (III.6) and (III.9)).

$$\boxed{\sigma_{\text{incoh}}^{(\text{inel})} = 4\pi A \left[\frac{c_0}{\omega_0^{\frac{1}{2}}} + c_1\,\omega_0^{\frac{1}{2}} + \cdots\right]} \qquad \text{(III.31)}$$

with

$$c_0 = \frac{\bar{\Delta}_0^{\frac{1}{2}}}{2\pi^{\frac{1}{2}}} \frac{(1+\frac{1}{4}x^2)^{\frac{1}{2}} - \frac{1}{2}x}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}} \left[(1+\bar{\gamma}_2 g_2)\frac{z}{1-z} + (h_1 + \bar{\gamma}_2 g_3)\ln\left(\frac{1}{1-z}\right) + \right.$$

$$\left. + \bar{\gamma}_2 g_1 \frac{z}{(1-z)^2}\right], \qquad \text{(III.31')}$$

$$c_1 = \frac{\bar{\Delta}_0^{\frac{1}{2}}}{2\pi^{\frac{1}{2}}} \frac{(1+\frac{1}{4}x^2)^{\frac{1}{2}} - \frac{1}{2}x}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}} \frac{1}{\bar{\Delta}_0} \left[p_1 \frac{z}{(1-z)^2} + p_2 \frac{z}{1-z} + p_3 \ln\left(\frac{1}{1-z}\right)\right]. \qquad \text{(III.31'')}$$

For $\beta \to 0$ $(T \to \infty)$ c_0 and c_1 tend to

$$c_0 \to \frac{2}{\mu^2 \pi^{\frac{1}{2}}} \left(\frac{m}{2 M \beta}\right)^{\frac{1}{2}}, \qquad c_1 \to \frac{2}{\mu^2 \pi^{\frac{1}{2}}} \frac{1}{3} \left(\frac{m}{2 M \beta}\right)^{-\frac{1}{2}}, \quad \mu = 1 + \frac{m}{M},$$

and (III.31) thus approaches the expression given in (II.17′).

Numerical comparisons

Accurate calculations of the total cross section have been made using Walker's frequency distribution for Al.(¹) The contribution from each phonon term is determined and these values are compared with those obtained from the approximate expressions (III.21) and (III.26). Two cases are considered, one with $T = 300°$K and one with $T = 74.8°$K (see Tables 3 a and 3 b). The separate terms in the m/M expansion are also calculated from formula (III.13′) and these values are in Table 4 compared with the values which are obtained from Placzek's expression for a Debye crystal (see ref. [7]). The Debye temperature is then defined from the Debye–Waller factor. For $(m/M)\,\bar{\gamma}\,(0)\,\bar{\Delta}_0$ we have taken the value 0.5.(²)

Table 3 a. $(T = 300°\mathrm{K})$

n	$\sigma_1^{(n)}$ (exact)	$\sigma_{1,0}^{(n)}$	$\sigma_{1,0}^{(n)} + \sigma_{1,1}^{(n)}$
1	0.05593	0.04849	0.05183
2	0.02046	0.01950	0.02044
3	0.00813	0.00784	0.00812
4	0.00323	0.00315	0.00323
5	0.001281	0.001267	0.001288
6	. . .	0.00051	0.00051
7	. . .	0.00020	0.00020
8	. . .	0.00008	0.00008
	0.0898	0.0810	0.0857

Table 3 b. $(T = 74.8°\mathrm{K})$

0_2502, for instance, means 0.00503.

n	$\sigma_1^{(n)}$ (exact)	$\sigma_{1,0}^{(n)}$	$\sigma_{1,0}^{(n)} + \sigma_{1,1}^{(n)}$
1	0_2502	0_2459	0_2478
2	0_3230	0_3224	0_3232
3	0_4115	0_4111	0_4114
4	0_6575	0_6563	0_6579
5	0_7288	0_7281	0_7288

(¹) This frequency spectrum is adopted only to get a realistic one for our comparisons.

(²) This case should for $T = 300°$K correspond to a hypothetical crystal with the mass ratio $M/m = 5.46$ and with the same frequency spectrum as Al.

Table 4. ($T = 300°K$)

	$\left[\frac{m}{M}\gamma(0)\right]^n \bar{\sigma}_n$	
n	exact	Placzek's approx.(¹)
1	+0.1017	+0.1019
2	−0.0062	−0.0071
3	−0.0069	—
4	+0.0012	—
	0.0898	0.0948

(¹) Placzek does not give more than two terms in the expansion.

APPENDIX I

The scattering cross section for neutrons colliding with free nuclei with a prescribed momentum distribution (1)

Consider first a neutron colliding with a free nucleus having the velocity $\dot{\boldsymbol{u}}$ before the collision. As previously the neutron energies before and after the collision are denoted by $\hbar\omega_0$ and $\hbar\omega$ respectively. The energy-momentum laws then give

$$\omega - \omega_0 + \frac{\hbar\varkappa^2}{2M} + (\boldsymbol{\varkappa}\cdot\dot{\mathbf{u}}) = 0 \qquad \text{(A-I.1)}$$

and the scattering cross section may be written

$$\frac{d^2\sigma}{d\Omega\, d\omega} = a^2\frac{k}{k_0}\,\delta\left(\omega - \omega_0 + \frac{\hbar\varkappa^2}{2M} + \boldsymbol{\varkappa}\cdot\dot{\mathbf{u}}\right), \qquad \text{(A-I.2)}$$

a being the bound scattering length for the nucleus. The Fourier-integral representation of the δ-function is introduced and the cross section is averaged over the prescribed velocity distribution of the nucleus, adopting the same distribution as found for the nucleus in the crystal considered. We get

$$\left(\frac{d^2\sigma}{d\Omega\, d\omega}\right)_{\text{Av}} = a^2\frac{k}{k_0}\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[i\left(\omega-\omega_0+\frac{\hbar\varkappa^2}{2M}\right)t\right]\langle\exp\left[i t(\boldsymbol{\varkappa}\cdot\dot{\mathbf{u}})\right]\rangle_T\, dt. \qquad \text{(A-I.3)}$$

In the harmonic approximation for the crystal vibrations this velocity distribution is a Gaussian one and we can then write

$$\langle\exp\left[i t(\boldsymbol{\varkappa}\cdot\dot{\mathbf{u}})\right]\rangle_T = \exp\left[-\frac{t^2}{2}\langle(\boldsymbol{\varkappa}\cdot\dot{\mathbf{u}})^2\rangle_T\right]. \qquad \text{(A-I.4)}$$

By differentiating $\langle\mathbf{u}(t')\,\mathbf{u}(t)\rangle_T$, explicitly given in (I.8), we can further show that

$$\langle(\boldsymbol{\varkappa}\cdot\dot{\mathbf{u}})^2\rangle_T = \frac{1}{NM}\sum_s \varepsilon_s\left|\boldsymbol{\varkappa}\cdot\mathbf{C}_s\right| = \frac{\hbar}{M}(\boldsymbol{\varkappa}\cdot\boldsymbol{\varepsilon}\cdot\boldsymbol{\varkappa}) \qquad \text{(A-I.5)}$$

and putting this into (A-I.3) the scattering cross section is written

$$\left(\frac{d^2\sigma}{d\Omega\, d\omega}\right)_{\text{Av}} = a^2\frac{k}{k_0}\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[i\left(\omega-\omega_0+\frac{\hbar\varkappa^2}{2M}\right)t\right]\exp\left[-\frac{t^2}{2}\frac{\hbar}{M}(\boldsymbol{\varkappa}\cdot\boldsymbol{\varepsilon}\cdot\boldsymbol{\varkappa})\right]dt.$$

(A-I.6)

This expression may now be transformed into the form given in (II.7).

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(1) Se also: G. F. von Dardel, Phys. Rev., *94*, 1274 (1954), part. D.

APPENDIX II

Tables of $\gamma(0)$, Δ_0, γ_1, γ_2 and related quantities, obtained in the Debye approximation

$$\beta_D = \frac{\hbar \omega_D}{2 k_B T}, \text{ where } \omega_D = \text{the Debye frequency.}$$

β_D	$\gamma_D(0)$	$\Delta_{0,D}$	β_1	$\gamma_D(0) \exp(-\beta_1^2/2)$	γ_1	γ_2
0.0	∞	0.577	0.000	∞	0.000	−0.050
0.1	30.030	0.577	0.052	29.998		
0.2	15.066	0.575	0.116	14.965	−0.023	−0.049
0.3	10.099	0.571	0.173	9.949		
0.4	7.632	0.566	0.231	7.431	−0.046	−0.045
0.5	6.165	0.560	0.289	5.912		
0.6	5.197	0.554	0.348	4.892	−0.067	−0.040
0.7	4.515	0.546	0.406	4.157		
0.8	4.010	0.537	0.464	3.600	−0.088	−0.032
0.9	3.624	0.528	0.523	3.161		
1.0	3.321	0.518	0.582	2.804	−0.107	−0.024
1.1	3.078	0.508	0.640	2.508		
1.2	2.879	0.497	0.699	2.255	−0.123	−0.014
1.3	2.715	0.486	0.757	2.038		
1.4	2.577	0.476	0.815	1.848	−0.138	−0.004
1.5	2.461	0.465	0.873	1.681		
1.6	2.362	0.455	0.931	1.532	−0.150	+0.005
1.7	2.276	0.445	0.987	1.398		
1.8	2.203	0.435	1.044	1.278	−0.160	+0.014
1.9	2.138	0.425	1.099	1.169		
2.0	2.082	0.416	1.154	1.070	−0.167	+0.021
2.5	1.885	0.376	1.411	0.697		
3.0	1.771	0.345	1.635	0.466	−0.175	+0.036
3.5	1.701	0.325	1.823	0.323		
4.0	1.654	0.306	1.978	0.234	−0.162	+0.028
4.5	1.622	0.293	2.104	0.177		
5.0	1.599	0.283	2.208	0.140	−0.147	+0.017
5.5	1.582	0.276	2.292	0.114		
6.0	1.569	0.270	2.361	0.097	−0.136	+0.006
∞	1.500	0.236	2.825	0.027	−0.094	−0.025

Tables of $\bar{\gamma}(0)$, $\overline{\Delta}_0$ *and* $\bar{\gamma}_2$, *obtained in the Debye approximation.*

β_D	$\bar{\gamma}_D(0)$	$\overline{\Delta}_{0,D}$	$\bar{\gamma}_2$
0.0	∞	0.577	−0.0500
0.1	29.982	0.577	
0.2	14.966	0.577	−0.0498
0.3	9.950	0.576	
0.4	7.434	0.575	−0.0497
0.5	5.918	0.574	
0.6	4.902	0.573	−0.0493
0.7	4.173	0.571	
0.8	3.622	0.569	−0.0488
0.9	3.191	0.567	
1.0	2.844	0.565	−0.0481
1.1	2.558	0.562	
1.2	2.318	0.560	−0.0473
1.3	2.114	0.557	
1.4	1.937	0.554	−0.0463
1.5	1.784	0.550	
1.6	1.648	0.547	−0.0453
1.7	1.529	0.543	
1.8	1.421	0.540	−0.0440
1.9	1.325	0.536	
2.0	1.239	0.532	−0.0427

Tabl

$$F(z, x) = \sum_{n=2}^{\infty} \frac{z^n}{n!} \frac{\exp(-x^2/2n}{(2\pi n)^{\frac{1}{2}}}$$

$x = 0.0, \dots$

x \ z	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.
0.0	0_2145	0_2596	0_1138	0_1253	0_1406	0_1603	0_1846	0.114	0.149	0.190	0.2
0.1	0_2145	0_2595	0_1138	0_1252	0_1405	0_1601	0_1844	0.114	0.148	0.189	0.2
0.2	0_2144	0_2591	0_1137	0_1250	0_1402	0_1597	0_1838	0.113	0.147	0.188	0.2
0.3	0_2142	0_2583	0_1135	0_1247	0_1398	0_1590	0_1828	0.112	0.146	0.186	0.2
0.4	0_2139	0_2573	0_1133	0_1243	0_1391	0_1580	0_1815	0.110	0.143	0.183	0.2
0.5	0_2136	0_2561	0_1130	0_1238	0_1383	0_1568	0_1798	0.108	0.140	0.179	0.2
0.6	0_2133	0_2546	0_1127	0_1232	0_1373	0_1554	0_1777	0.105	0.137	0.175	0.2
0.7	0_2128	0_2529	0_1123	0_1225	0_1362	0_1537	0_1754	0.102	0.133	0.170	0.2
0.8	0_2124	0_2510	0_1118	0_1217	0_1349	0_1518	0_1728	0_1983	0.129	0.164	0.2
0.9	0_2119	0_2489	0_1113	0_1208	0_1335	0_1498	0_1700	0_1945	0.124	0.158	0.1
1.0	0_2113	0_2467	0_1108	0_1199	0_1320	0_1476	0_1670	0_1905	0.118	0.151	0.1
1.1	0_2107	0_2443	0_1103	0_1189	0_1305	0_1453	0_1638	0_1862	0.113	0.144	0.1
1.2	0_2102	0_2419	0_2973	0_1179	0_1289	0_1430	0_1605	0_1818	0.107	0.137	0.1
1.3	0_3954	0_2394	0_2916	0_1168	0_1272	0_1405	0_1571	0_1772	0.101	0.130	0.1
1.4	0_3892	0_2369	0_2858	0_1158	0_1255	0_1380	0_1536	0_1726	0_1953	0.122	0.1
1.5	0_3831	0_2344	0_2800	0_1147	0_1238	0_1356	0_1502	0_1680	0_1893	0.114	0.1
1.6	0_3769	0_2319	0_2742	0_1137	0_1221	0_1331	0_1467	0_1633	0_1833	0.107	0.1
1.7	0_3709	0_2294	0_2685	0_1126	0_1205	0_1306	0_1433	0_1588	0_1773	0_1993	0.1
1.8	0_3650	0_2270	0_2630	0_1116	0_1189	0_1282	0_1400	0_1543	0_1715	0_1919	0.1
1.9	0_3594	0_2247	0_2576	0_1107	0_1173	0_1259	0_1367	0_1499	0_1659	0_1848	0.1
2.0	0_3539	0_2224	0_2525	0_2970	0_1158	0_1237	0_1336	0_1457	0_1604	0_1778	0_19
2.1	0_3487	0_2203	0_2475	0_2880	0_1143	0_1215	0_1306	0_1417	0_1552	0_1712	0_19
2.2	0_3438	0_2183	0_2429	0_2795	0_1130	0_1195	0_1278	0_1379	0_1502	0_1648	0_18
2.3	0_3392	0_2164	0_2385	0_2715	0_1117	0_1176	0_1251	0_1343	0_1455	0_1588	0_17
2.4	0_3349	0_2146	0_2344	0_2640	0_1105	0_1158	0_1226	0_1309	0_1410	0_1532	0_16
2.5	0_3310	0_2130	0_2306	0_2570	0_2935	0_1141	0_1202	0_1277	0_1369	0_1479	0_16
2.6	0_3273	0_2115	0_2271	0_2506	0_2831	0_1126	0_1180	0_1248	0_1331	0_1429	0_15
2.7	0_3240	0_2101	0_2239	0_2447	0_2736	0_1112	0_1160	0_1221	0_1295	0_1384	0_14
2.8	0_3209	0_3883	0_2210	0_2393	0_2648	0_2986	0_1142	0_1196	0_1262	0_1342	0_14
2.9	0_3182	0_3770	0_2183	0_2344	0_2569	0_2868	0_1125	0_1173	0_1232	0_1304	0_13
3.0	0_3158	0_3668	0_2159	0_2300	0_2498	0_2760	0_1110	0_1152	0_1205	0_1269	0_13
3.1	0_3136	0_3577	0_2138	0_2261	0_2433	0_2644	0_2962	0_1134	0_1180	0_1237	0_13
3.2	0_3116	0_3496	0_2119	0_2226	0_2376	0_2578	0_2839	0_1117	0_1158	0_1208	0_12
3.3	0_4992	0_3424	0_2102	0_2194	0_2325	0_2501	0_2729	0_1102	0_1138	0_1183	0_22
3.4	0_4842	0_3362	0_3874	0_2167	0_2280	0_2432	0_2632	0_2886	0_1120	0_1160	0_12
3.5	0_4711	0_3307	0_3744	0_2143	0_2240	0_2372	0_2546	0_2768	0_1105	0_1139	0_11
3.6	0_4598	0_3259	0_3631	0_2121	0_2205	0_2319	0_2470	0_2663	0_2907	0_1121	0_11
3.7	0_4501	0_3218	0_3533	0_2103	0_2175	0_2273	0_2403	0_2571	0_2784	0_1105	0_11
3.8	0_4418	0_3183	0_3449	0_3871	0_2148	0_2233	0_2345	0_2491	0_2676	0_2907	0_11
3.9	0_4346	0_3152	0_3376	0_3734	0_2126	0_2198	0_2295	0_2421	0_2581	0_2783	0_11
4.0	0_4286	0_3127	0_3314	0_3616	0_2106	0_2168	0_2251	0_2360	0_2499	0_2675	0_28
4.1	0_4235	0_3105	0_3262	0_3516	0_3892	0_2142	0_2213	0_2307	0_2427	0_2580	0_27
4.2	0_4193	0_4864	0_3217	0_3431	0_3748	0_2120	0_2181	0_2261	0_2365	0_2498	0_26
4.3	0_4157	0_4709	0_3180	0_3358	0_3626	0_2101	0_2153	0_2222	0_2312	0_2426	0_25
4.4	0_4128	0_4581	0_3148	0_3297	0_3523	0_3845	0_2129	0_2188	0_2265	0_2365	0_24
4.5	0_4103	0_4473	0_3122	0_3246	0_3436	0_3708	0_2109	0_2159	0_2226	0_2311	0_24
4.6						0_3592	0_3913	0_2135	0_2192	0_2266	0_23
4.7						0_3494	0_3766	0_2114	0_2163	0_2226	0_23
4.8						0_3412	0_3642	0_3957	0_2138	0_2192	0_22
4.9						0_3343	0_3538	0_3805	0_2116	0_2164	0_22
5.0						0_3285	0_3450	0_3677	0_3984	0_2139	0_21
5.1											
5.2											
5.3											
5.4											

$x)$

$z)^{\frac{1}{2}} \exp\left(z-\frac{x^2}{2z}\right), \quad z\to\infty.$

.1, … 4.4

.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2
291	0.353	0.424	0.504	0.593	0.694	0.806	0.932	1.071	1.226	1.398
291	0.353	0.423	0.502	0.592	0.692	0.805	0.930	1.069	1.224	1.396
289	0.350	0.420	0.500	0.588	0.688	0.800	0.924	1.063	1.221	1.387
285	0.346	0.416	0.494	0.582	0.681	0.791	0.915	1.052	1.205	1.374
281	0.341	0.409	0.487	0.574	0.671	0.780	0.902	1.037	1.188	1.355
276	0.335	0.402	0.477	0.563	0.659	0.766	0.886	1.019	1.167	1.332
269	0.327	0.392	0.466	0.550	0.644	0.749	0.866	0.997	1.142	1.303
261	0.318	0.381	0.454	0.535	0.627	0.729	0.844	0.971	1.113	1.271
253	0.307	0.369	0.439	0.519	0.607	0.707	0.818	0.943	1.081	1.235
244	0.296	0.356	0.424	0.500	0.586	0.683	0.791	0.911	1.046	1.195
234	0.284	0.342	0.407	0.481	0.564	0.657	0.761	0.878	1.007	1.152
223	0.272	0.327	0.390	0.460	0.540	0.630	0.730	0.842	0.967	1.106
212	0.258	0.311	0.371	0.439	0.515	0.601	0.697	0.805	0.925	1.059
201	0.245	0.295	0.352	0.417	0.490	0.572	0.663	0.766	0.881	1.009
190	0.231	0.279	0.333	0.394	0.463	0.541	0.629	0.727	0.837	0.959
178	0.217	0.262	0.313	0.371	0.437	0.511	0.594	0.687	0.791	0.908
166	0.203	0.246	0.294	0.349	0.411	0.480	0.559	0.647	0.746	0.857
155	0.190	0.229	0.274	0.326	0.384	0.450	0.524	0.607	0.701	0.805
144	0.176	0.213	0.255	0.304	0.358	0.420	0.490	0.568	0.656	0.755
133	0.163	0.197	0.237	0.282	0.333	0.391	0.456	0.530	0.612	0.705
122	0.150	0.182	0.219	0.261	0.308	0.362	0.423	0.492	0.569	0.656
112	0.138	0.167	0.201	0.240	0.284	0.335	0.391	0.456	0.528	0.609
102	0.126	0.153	0.185	0.220	0.261	0.308	0.361	0.421	0.488	0.564
932	0.115	0.140	0.169	0.202	0.240	0.283	0.332	0.387	0.450	0.520
845	0.104	0.127	0.154	0.184	0.219	0.259	0.304	0.355	0.413	0.479
763	0_1943	0.115	0.140	0.167	0.199	0.236	0.278	0.325	0.379	0.439
687	0_1851	0.104	0.126	0.152	0.181	0.215	0.253	0.296	0.346	0.402
617	0_1765	0_1938	0.114	0.137	0.164	0.195	0.230	0.270	0.315	0.367
552	0_1685	0_1842	0.102	0.124	0.148	0.176	0.208	0.245	0.287	0.334
$_1492$	0_1612	0_1754	0_1919	0.111	0.133	0.159	0.188	0.222	0.260	0.303
$_1437$	0_1545	0_1673	0_1822	0_1995	0.120	0.143	0.169	0.200	0.235	0.275
$_1387$	0_1484	0_1599	0_1733	0_1889	0.107	0.128	0.152	0.180	0.212	0.249
$_1342$	0_1429	0_1532	0_1652	0_1793	0_1957	0.115	0.137	0.162	0.191	0.225
$_1301$	0_1379	0_1471	0_1579	0_1705	0_1853	0.103	0.122	0.145	0.172	0.202
$_1265$	0_1334	0_1416	0_1512	0_1626	0_1759	0_1914	0.109	0.130	0.154	0.182
$_1232$	0_1293	0_1366	0_1453	0_1555	0_1674	0_1813	0_1975	0.116	0.138	0.163
$_1203$	0_1257	0_1322	0_1399	0_1490	0_1597	0_1722	0_1868	0.104	0.124	0.146
$_1177$	0_1225	0_1283	0_1351	0_1432	0_1528	0_1640	0_1772	0_1925	0.110	0.131
$_1154$	0_1197	0_1248	0_1308	0_1381	0_1466	0_1567	0_1685	0_1822	0_1982	0.117
$_1134$	0_1171	0_1216	0_1270	0_1335	0_1411	0_1501	0_1607	0_1730	0_1874	0.104
$_1116$	0_1149	0_1189	0_1237	0_1294	0_1362	0_1442	0_1537	0_1647	0_1777	0_1928
$_1101$	0_1130	0_1165	0_1207	0_1258	0_1318	0_1390	0_1474	0_1573	0_1690	0_1826
$_2870$	0_1112	0_1143	0_1181	0_1225	0_1279	0_1343	0_1418	0_1507	0_1612	0_1734
$_2751$	0_2973	0_1124	0_1157	0_1197	0_1245	0_1301	0_1369	0_1448	0_1542	0_1651
$_2647$	0_2841	0_1108	0_1137	0_1172	0_1214	0_1265	0_1324	0_1395	0_1479	0_1577
$_2557$	0_2727	0_2936	0_1119	0_1150	0_1187	0_1232	0_1285	0_1349	0_1423	0_1511
$_2479$	0_2627	0_2810	0_1103	0_1131	0_1164	0_1203	0_1251	0_1307	0_1374	0_1453
$_2411$	0_2540	0_2700	0_2897	0_1114	0_1143	0_1178	0_1220	0_1270	0_1330	0_1400
$_2353$	0_2465	0_2605	0_2778	0_2989	0_1125	0_1156	0_1193	0_1237	0_1290	0_1353
$_2302$	0_2400	0_2522	0_2673	0_2859	0_1109	0_1136	0_1169	0_1208	0_1256	0_1312
$_2259$	0_2344	0_2450	0_2583	0_2745	0_2944	0_1119	0_1148	0_1183	0_1225	0_1275
					0_2821	0_1104	0_1129	0_1160	0_1198	0_1242
					0_2714	0_2902	0_1113	0_1141	0_1174	0_1213
					0_2620	0_2785	0_2986	0_1123	0_1152	0_1188
					0_2538	0_2683	0_2861	0_1108	0_1134	0_1165

(*contd.*)

$x \backslash z$	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2
0.0	1.589	1.799	2.032	2.288	2.571	2.883	3.226	3.604	4.019	4.475
0.2	1.577	1.786	2.017	2.272	2.553	2.862	3.203	3.579	3.991	4.445
0.4	1.540	1.745	1.972	2.222	2.497	2.801	3.136	3.504	3.910	4.355
0.6	1.482	1.680	1.899	2.141	2.408	2.703	3.027	3.384	3.778	4.210
0.8	1.405	1.594	1.803	2.034	2.289	2.571	2.882	3.224	3.600	4.017
1.0	1.312	1.490	1.687	1.905	2.146	2.412	2.706	3.031	3.388	3.783
1.2	1.207	1.372	1.556	1.759	1.984	2.233	2.508	2.812	3.147	3.517
1.4	1.095	1.247	1.415	1.602	1.810	2.040	2.294	2.575	2.887	3.231
1.6	0.980	1.117	1.270	1.441	1.630	1.840	2.072	2.330	2.616	2.932
1.8	0.865	0.988	1.126	1.279	1.450	1.639	1.850	2.084	2.344	2.631
2.0	0.754	0.863	0.985	1.122	1.274	1.444	1.633	1.843	2.077	2.336
2.2	0.649	0.745	0.853	0.973	1.107	1.258	1.426	1.613	1.821	2.053
2.4	0.553	0.636	0.730	0.835	0.952	1.084	1.232	1.397	1.581	1.787
2.6	0.465	0.537	0.618	0.709	0.811	0.926	1.055	1.199	1.361	1.542
2.8	0.388	0.449	0.518	0.596	0.685	0.784	0.895	1.021	1.162	1.320
3.0	0.321	0.372	0.431	0.498	0.573	0.658	0.754	0.862	0.984	1.121
3.2	0.263	0.306	0.356	0.412	0.476	0.548	0.630	0.723	0.827	0.945
3.4	0.214	0.250	0.291	0.339	0.392	0.454	0.523	0.602	0.691	0.792
3.6	0.172	0.202	0.237	0.277	0.322	0.373	0.432	0.498	0.574	0.660
3.8	0.138	0.163	0.192	0.225	0.262	0.305	0.354	0.411	0.474	0.547
4.0	0.110	0.131	0.154	0.181	0.213	0.248	0.289	0.336	0.390	0.451
4.2	0_1876	0.104	0.124	0.146	0.171	0.201	0.235	0.274	0.319	0.371
4.4	0_1693	0_1827	0_1984	0.117	0.138	0.162	0.190	0.223	0.260	0.303
4.6	0_1545	0_1654	0_1781	0_1930	0.110	0.130	0.154	0.180	0.211	0.247
4.8	0_1428	0_1515	0_1618	0_1738	0_1879	0.104	0.123	0.145	0.171	0.200
5.0	0_1334	0_1404	0_1487	0_1584	0_1698	0_1831	0_1986	0.117	0.138	0.162
5.2	0_1260	0_1316	0_1383	0_1461	0_1553	0_1661	0_1787	0_1934	0.111	0.131
5.4	0_1202	0_1247	0_1300	0_1362	0_1436	0_1523	0_1626	0_1745	0_1885	0.105
5.6	0_1157	0_1192	0_1234	0_1284	0_1343	0_1413	0_1496	0_1593	0_1706	0_1839
5.8	0_1121	0_1149	0_1182	0_1222	0_1269	0_1326	0_1392	0_1470	0_1562	0_1670
6.0	0_2930	0_1115	0_1141	0_1173	0_1211	0_1256	0_1309	0_1372	0_1446	0_1533
6.2	0_2714	0_2887	0_1109	0_1134	0_1164	0_1200	0_1243	0_1293	0_1353	0_1423
6.4	0_2547	0_2682	0_2845	0_1104	0_1128	0_1156	0_1190	0_1230	0_1278	0_1335
6.6	0_2418	0_2523	0_2651	0_2805	0_2992	0_1122	0_1149	0_1181	0_1219	0_1264
6.8	0_2318	0_2400	0_2500	0_2621	0_2768	0_2945	0_1116	0_1141	0_1172	0_1208
7.0	0_2242	0_2305	0_2383	0_2478	0_2593	0_2732	0_2900	0_1110	0_1134	0_1163
7.2										
7.4										
7.6										
7.8										
8.0										

.4	3.5	3.6	3.7	3.8	3.9	4.0	4.1	4.2	4.3	4.4
527	6.131	6.795	7.523	8.322	9.199	10.16	11.22	12.37	13.64	15.03
491	6.092	6.752	7.476	8.271	9.143	10.10	11.15	12.30	13.56	14.95
383	5.974	6.624	7.336	8.119	8.977	9.920	10.95	12.09	13.33	14.70
210	5.785	6.416	7.110	7.872	8.709	9.628	10.64	11.74	12.96	14.29
977	5.530	6.139	6.807	7.542	8.349	9.236	10.21	11.28	12.46	13.75
696	5.222	5.802	6.439	7.141	7.912	8.760	9.692	10.72	11.84	13.08
376	4.872	5.418	6.020	6.683	7.413	8.216	9.100	10.07	11.14	12.32
030	4.492	5.003	5.566	6.186	6.870	7.623	8.454	9.368	10.37	11.48
669	4.096	4.568	5.089	5.665	6.300	7.001	7.774	8.627	9.567	10.60
304	3.695	4.127	4.606	5.135	5.720	6.366	7.080	7.869	8.740	9.701
944	3.299	3.692	4.128	4.610	5.144	5.736	6.390	7.113	7.913	8.798
598	2.917	3.272	3.665	4.101	4.585	5.122	5.717	6.376	7.105	7.913
272	2.557	2.873	3.226	3.618	4.053	4.536	5.073	5.669	6.330	7.063
970	2.222	2.503	2.816	3.166	3.554	3.987	4.468	5.003	5.598	6.259
695	1.916	2.164	2.441	2.750	3.094	3.479	3.908	4.385	4.917	5.508
477	1.641	1.857	2.100	2.372	2.676	3.016	3.395	3.818	4.291	4.818
227	1.395	1.584	1.796	2.034	2.300	2.598	2.932	3.305	3.723	4.189
035	1.180	1.343	1.527	1.733	1.965	2.226	2.518	2.845	3.212	3.623
867	0.992	1.132	1.291	1.469	1.670	1.896	2.151	2.436	2.757	3.117
723	0.830	0.950	1.086	1.239	1.413	1.608	1.828	2.076	2.355	2.669
600	0.691	0.793	0.909	1.040	1.189	1.357	1.547	1.761	2.003	2.275
496	0.572	0.659	0.758	0.870	0.997	1.141	1.303	1.488	1.696	1.931
408	0.472	0.546	0.629	0.724	0.832	0.955	1.094	1.251	1.430	1.632
335	0.388	0.450	0.520	0.600	0.692	0.796	0.914	1.049	1.201	1.374
273	0.318	0.370	0.429	0.496	0.573	0.661	0.761	0.875	1.005	1.153
222	0.260	0.303	0.352	0.408	0.473	0.547	0.632	0.728	0.838	0.964
180	0.211	0.247	0.288	0.335	0.389	0.451	0.522	0.604	0.697	0.803
146	0.171	0.201	0.235	0.274	0.319	0.371	0.430	0.499	0.577	0.666
117	0.138	0.163	0.191	0.223	0.261	0.304	0.354	0.411	0.476	0.552
943	0.111	0.131	0.155	0.181	0.212	0.248	0.290	0.337	0.392	0.455
755	0_1895	0.106	0.125	0.147	0.173	0.202	0.237	0.276	0.322	0.374
603	0_1717	0_1850	0.101	0.119	0.140	0.164	0.193	0.225	0.263	0.307
480	0_1573	0_1681	0_1808	0_1956	0.113	0.133	0.156	0.183	0.215	0.251
381	0_1456	0_1544	0_1647	0_1768	0_1909	0.107	0.127	0.149	0.175	0.205
302	0_1362	0_1433	0_1517	0_1615	0_1730	0_1865	0.102	0.120	0.142	0.167
239	0_1287	0_1344	0_1412	0_1492	0_1585	0_1694	0_1823	0_1972	0.115	0.135
188	0_1227	0_1273	0_1328	0_1392	0_1468	0_1556	0_1661	0_1783	0_1926	0.109
148	0_1179	0_1216	0_1260	0_1312	0_1373	0_1445	0_1530	0_1629	0_1746	0_1882
116	0_1141	0_1170	0_1205	0_1247	0_1296	0_1355	0_1423	0_1504	0_1599	0_1710
908	0_1111	0_1134	0_1162	0_1196	0_1235	0_1282	0_1338	0_1403	0_1480	0_1570
709	0_2865	0_1105	0_1128	0_1154	0_1186	0_1224	0_1269	0_1321	0_1384	0_1457

APPENDIX III

Approximate expressions of the Weber–Hermite functions (¹)

The Weber–Hermite functions $D_{-(n+\frac{1}{2})}(x\sqrt{n})$ satisfy the following differential equation:

$$y''(x) - n^2\left(1+\frac{x^2}{4}\right) y(x) = 0, \tag{A-III.1}$$

and as we are especially concerned with rather large values of $n\,(n \geqslant 2)$ we can use the WKB method to obtain approximate expressions for these functions. According to this method a new function $u(x)$ is defined by

$$y(x) = \exp\left(n\int_0^x u(t)\,dt\right) \tag{A-III.2}$$

and this satisfies the equation below

$$\frac{1}{n}u' = 1+\frac{x^2}{4} - u^2. \tag{A-III.3}$$

If $u(x)$ is now expanded into powers of $1/n$

$$u(x) = \sum_k n^{-k}\, u_k(x). \tag{A-III.4}$$

u_k are determined from the following recursion formulae:

$$\left.\begin{aligned} u_0^2 &= 1+\tfrac{1}{4}x^2, \\ u_0' + 2u_0u_1 &= 0, \\ u_1' + 2u_0u_2 + u_1^2 &= 0, \\ u_2' + 2u_0u_3 + 2u_1u_2 &= 0, \\ \cdots &\cdots\cdots\cdots \end{aligned}\right\} \tag{A-III.5}$$

and it is a straightforward matter to derive the solutions. The first few of these are given below.

(¹) The properties of these functions are briefly discussed in e.g. Erdelyi, Magnus, Oberhettinger, and Tricomi, Higher Transcendental Functions, vol. 2, pp. 116–130, New York 1953. See also: N. Schwid, Trans. Amer. Math. Soc., *37*, 339 (1935).

$$\left.\begin{aligned} u_0 &= \pm\left(1+\frac{x^2}{4}\right)^{\frac{1}{2}}, \\ u_1 &= \frac{d}{dx}\left[\ln\left(1+\frac{x^2}{4}\right)^{-\frac{1}{4}}\right], \\ u_2 &= \mp\frac{1}{32}\left[3\left(1+\frac{x^2}{4}\right)^{-\frac{3}{2}} - 5\left(1+\frac{x^2}{4}\right)^{-\frac{5}{2}}\right], \\ u_3 &= -\frac{3}{32}\,\frac{x}{2}\left[\left(1+\frac{x^2}{4}\right)^{-3} - \frac{5}{2}\left(1+\frac{x^2}{4}\right)^{-4}\right], \\ & \ldots\ldots\ldots\ldots\ldots\ldots \end{aligned}\right\} \tag{A-III.6}$$

The original function $y(x)$ is then obtained in the form

$$y(x) = \frac{\text{const}}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}}\exp\left[\pm n\int_0^x\left(1+\frac{t^2}{4}\right)^{\frac{1}{2}}dt + \frac{1}{n}\int_0^x u_2(t)\,dt + \frac{1}{n^2}\int_0^x u_3(t)\,dt + \cdots\right]. \tag{A-III.7}$$

The ± signs correspond to two independent solutions, and we must specify both the sign and the constant factor to get an approximation for $D_{-(n+\frac{1}{2})}(x\sqrt{n})$. For this purpose we let $x \to \infty$, where (A-III.7) tends to

$$y(x) \to \text{const}\,\sqrt{2}\,e^c\left(\sqrt{n}\right)^{\frac{1}{2}\mp n}\left(x\sqrt{n}\right)^{-\frac{1}{2}\pm n}\exp\left(\pm\frac{n x^2}{4}\right) \tag{A-III.8}$$

with
$$c = \pm\frac{n}{2} + \frac{1}{n}\int_0^\infty u_2(t)\,dt + \frac{1}{n^2}\int_0^\infty u_3(t)\,dt + \cdots.$$

This expression should be compared with the corresponding one for $D_{-(n+\frac{1}{2})}(x\sqrt{n})$(¹)

$$D_{-(n+\frac{1}{2})}(x\sqrt{n}) \to (x\sqrt{n})^{-(n+\frac{1}{2})}\,e^{-nx^2/4} \tag{A-III.9}$$

leading us to conclude that the lower sign should be chosen and that the constant factor must be

$$\text{const} = 2^{-\frac{1}{2}}\,e^{-c}\left(\sqrt{n}\right)^{-(n+\frac{1}{2})}. \tag{A-III.10}$$

To obtain a more convenient expression we finally expand in powers of $1/n$, where we get

$$\boxed{D_{-(n+\frac{1}{2})}(x\sqrt{n}) = \frac{2^{-\frac{1}{2}}\left(\sqrt{n}\right)^{-(n+\frac{1}{2})}}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}}\exp\left[-n\left(\frac{x^2}{4}+f(x)\right)\right]\left\{1+\frac{1}{n}\varphi_1(x)+\cdots\right\}} \tag{A-III.11}$$

(¹) See: Erdelyi *et al.*, loc. cit., p. 122.

where

$$\left.\begin{aligned} f(x) &= -\frac{1}{2}\left[\left(1+\frac{x^2}{4}\right)^{\frac{1}{2}}-\frac{x}{2}\right]^2 - \ln\left[\left(1+\frac{x^2}{4}\right)^{\frac{1}{2}}-\frac{x}{2}\right], \\ \varphi_1(x) &= \frac{1}{96}\left[2 - x\left(1+\frac{x^2}{4}\right)^{-\frac{1}{2}} - 5x\left(1+\frac{x^2}{4}\right)^{-\frac{3}{2}}\right]. \end{aligned}\right\} \qquad \text{(A-III.11')}$$

A corresponding approximate expression for $D_{-(n+\frac{3}{2})}(x\sqrt{n})$ is obtained from (A-III.11) by using the relation

$$\left(n+\frac{1}{2}\right) D_{-(n+\frac{3}{2})}(z) = -\exp\left(-\frac{1}{4}z^2\right)\frac{d}{dz}\left[\exp\left(\frac{1}{4}z^2\right) D_{-(n+\frac{1}{2})}(z)\right]. \qquad \text{(A-III.12)}$$

We get

$$\boxed{\begin{aligned} D_{-(n+\frac{3}{2})}(x\sqrt{n}) = \frac{2^{-\frac{1}{2}}(\sqrt{n})^{-(n+\frac{1}{2})}}{(1+\frac{1}{4}x^2)^{\frac{1}{4}}}\left[\left(1+\frac{x^2}{4}\right)^{\frac{1}{2}}-\frac{x}{2}\right]\exp\left[-n\left(\frac{x^2}{4}+f(x)\right)\right]\frac{n^{\frac{1}{2}}}{n+\frac{1}{2}}\times \\ \times\left\{1+\frac{1}{n}\chi_1(x)+\cdots\right\} \end{aligned}} \qquad \text{(A-III.13)}$$

with

$$\chi_1(x) = \varphi_1(x) + \frac{1}{8}\,\frac{x\left[(1+\frac{1}{4}x^2)^{\frac{1}{2}}+\frac{1}{2}x\right]}{1+\frac{1}{4}x^2}. \qquad \text{(A-III.13')}$$

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(¹) There is an unfortunate misprint in the normalization of the polarization vector in the footnote on page 205. Should be: $|\mathbf{C}_s|^2 = \frac{1}{2}$.

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